3rd Edition

MATERIALS SCIENCE AND ENGINEERING AND THEIR IMPACT ON THE ENVIRONMENT

ICMSE

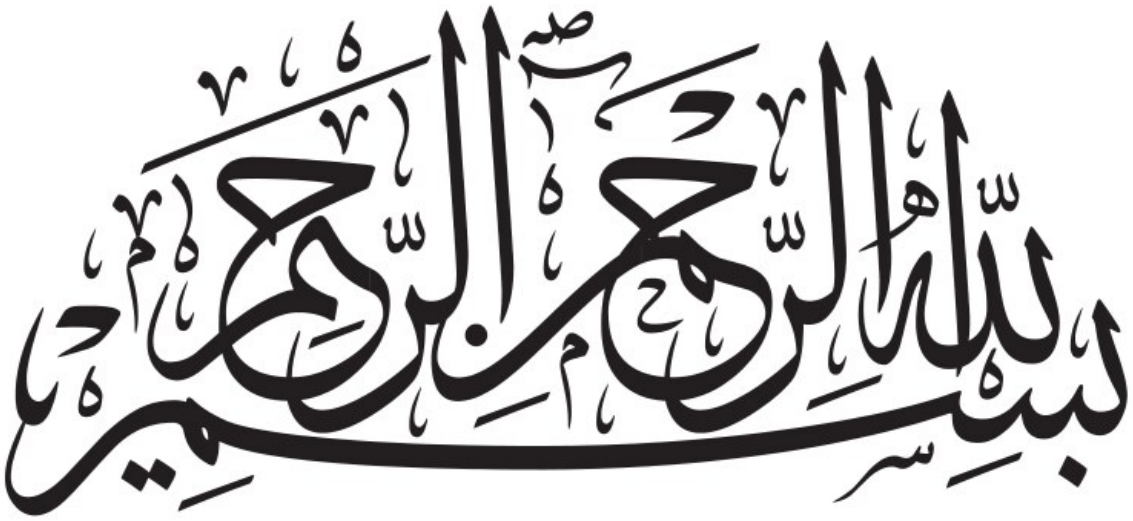
PROCEEDINGS BOOK

ISSN 2992-1694

Organized by Physico-Chemistry Laboratory Of Advanced Materials

May 29-30 / 2024 | HOTEL EDEN SIDI-BEL-ABBES

www.univ-sba.dz/lpcma/icmse2024


بسم الله الرحمن الرحيم

FOREWORD

ICMSE2024

This third edition of the International Conference on Materials Science and Engineering and their Impact on the Environment (ICMSE@2024) will be organized by the Laboratory of Physico-Chemistry of Advanced Materials (LPCMA) at Djillali Liabés University in Sidi Bel-Abbès. ICMSE@2024 provides an opportunity to promote communication between scientists and industry professionals to exchange information, ideas, and experiences in the development of new and innovative approaches to materials and their applications in energy and renewable energies, materials science and engineering, environment and sustainable development, biotechnology, and electrical engineering. The goal of the conference on materials science and engineering and their impact on the environment (ICMSE@2024) is to provide expert information on recent advances in key areas of materials science and engineering. Computational methods in materials science offer powerful support tools for making decisions regarding material choices and designs that meet specific application requirements in studies related to energy, nanotechnology, and materials. This meeting, aiming to take stock of the current state of research in the field of materials science, will be an opportunity to develop fruitful collaborations and partnerships among researchers, academics, and industry professionals

Importance of the Topic

This conference will focus on the latest interdisciplinary research in the prediction of new materials to address the challenges in energy, climate change, and environmental protection. It serves as a crucial event for senior and young researchers, students, and industry professionals working in this field worldwide.

Our Objective

This third international conference on materials science and engineering and their impact on the environment will facilitate a scientific gathering bringing together researchers and industry professionals at both national and international levels. The primary goal of this event is to foster the exchange of new studies and findings through plenary sessions, oral presentations, and posters. All scheduled presentations aim to initiate scientific discussions on the selection of materials with low environmental impact and environmentally friendly characteristics. This event combines modeling, simulation, and experimental approaches, drawing upon robust multidisciplinary expertise in physics, chemistry, physicochemistry of materials, process engineering, heat transfer, fluid dynamics, electrical engineering, meteorology, applied mathematics, and statistics.

SCIENTIFIC COMMITTEE

1.	**AMERI MOHAMMED**	**Pr**	**Univ. Of Sidi Bel-Abbés**
2.	**BOUZIANI MERAHI**	**Pr**	**Univ. Of Sidi Bel-Abbés**
3.	**BOUHAFS BACHIR**	**Pr**	**Univ. Of Sidi Bel-Abbés**
4.	**HARRACHE DJAMILA**	**Pr**	**Univ. Of Sidi Bel-Abbés**
5.	**BOUALEM ABIDRI**	**Pr**	**Univ. Of Sidi Bel-Abbés**
6.	**BENZAIR ABDENNOUR**	**Pr**	**Univ. Of Sidi Bel-Abbés**
7.	**BENKHETTOU NOUREDDINNE**	**Pr**	**Univ. Of Sidi Bel-Abbés**
8.	**RACHED DJAMEL**	**Pr**	**Univ. Of Sidi Bel-Abbés**
9.	**YARUB AL-DOURI**	**Pr**	**Univ. Of Malaya**
10.	**BOUYAKOUB ZAHIRA**	**Pr**	**Univ. Of Sidi Bel-Abbés**
11.	**DJEBARI ALI**	**Pr**	**Univ. Of Sidi Bel-Abbés**
12.	**DRIZ SAMIA**	**MCA**	**Univ. Of Sidi Bel-Abbés**
13.	**FASSI BENATTOU**	**MCA**	**Univ. Of Sidi Bel-Abbés**
14.	**HIRECH HOUARI**	**Pr**	**Univ. Of Sidi Bel-Abbés**
15.	**BOUKLI HACENE AMINE**	**Pr**	**Univ. Of Sidi Bel-Abbés**
16.	**ABROUCHE OMAR**	**Pr**	**Univ. Of SAIDA**
17.	**MESBAH SMAIN**	**MCA**	**Univ. Of Relizane**
18.	**BENGHAREZ DJAMILA**	**Pr**	**Univ. Of Sidi Bel-Abbés**
19.	**JELLALI SALAH**	**Pr**	**Sultan Qaboos University, Oman**
20.	**MATTHEUS GOOSEN**	**Pr**	**Alfaisal University, Saudi Arabia**
21.	**TAYEBI NADJIA**	**MCA**	**Univ. Of Sidi Bel-Abbés**
25.	**ROMDHANE SAMIR**	**Pr**	**Faculty of Sciences of Tunis**
26.	**LABIDI SALIMA**	**Pr**	**Univ. Of Annaba**
27.	**AL AHMAR SID AHMED**	**Pr**	**Univ. Of Sidi Bel-Abbés**
28.	**SLAHEDDINE OUNISSI**	**Pr**	**Centre Universitaire Of bayedh**
29.	**BOUZOUIRA NOUREDDINE**	**MCA**	**Centre Universitaire Of bayedh**
30.	**BOUAYAD LINDA**	**MCA**	**Univ. Of Sidi Bel-Abbés**
31.	**HACENE MAHMOUDI**	**Pr**	**Univ. Hassiba Benbouali Of Chlef, Algeria**
32.	**RABHI Abbes Aboubak**	**Pr**	**Univ. Of Sidi Bel-Abbés**
33.	**CHIALI CHARIF KHADIDJA**	**MCA**	**Univ. Of Sidi Bel-Abbés**

ORGANIZING COMMITTEE

1.	**AMERI MOHAMMED**	**Pr**	**Univ. Of Sidi Bel-Abbés**
2.	**CHIALI CHARIF KHADIDJA**	**MCA**	**Univ. Of Sidi Bel-Abbés**
3.	**MESBAH SMAIN**	**MCA**	**Univ. Of Sidi Bel-Abbés**
4.	**HARRACHE DJAMILA**	**Pr**	**Univ. Of Sidi Bel-Abbés**
5.	**TAYEBI NADJIA**	**MCA**	**Univ. Of Sidi Bel-Abbés**
6.	**CHEKROUN MED ZOHEIR**	**MCA**	**Univ. Of Sidi Bel-Abbés**
7.	**OUHIB RACHID**	**MCB**	**Univ. Of Sidi Bel-Abbés**
8.	**MOULESSEHOUL ATIKA**	**MCB**	**Univ. Oran 2**
9.	**DINE EL HENNANI MOHAMMED**	**MCA**	**Univ. Of Ain Temouchent**
10.	**BOUYAKOUB ZAHIRA**	**MCA**	**Univ. Of Sidi Bel-Abbés**
11.	**DRIZ SAMIA**	**MCA**	**Univ. Of Sidi Bel-Abbés**
12.	**FASSI BENATTOU**	**MCA**	**Univ. Of Sidi Bel-Abbés**
13.	**BOUZOUIRA NOUREDDINE**	**MCA**	**Centre Universitaire Of Bayedh**
14.	**BELDI LILIA**	**MCA**	**Univ. Of Sidi Bel-Abbés**
15.	**BOUAYAD LINDA**	**MCA**	**Univ. Of Sidi Bel-Abbés**
16.	**RAMDANI NADIA**	**Pr**	**Univ. Of Sidi Bel-Abbés**
17.	**ABID HAMZA**	**Pr**	**Univ. Of Sidi Bel-Abbés**
18.	**BENGHAREZ DJAMILA**	**Pr**	**Univ. Of Sidi Bel-Abbés**
19.	**KHATIR RADJA**	**MCA**	**ESGEE Oran**
20.	**BLAHA LAMIA FARAH**	**MAB**	**USTHB Alger**
21.	**AMERI IBRAHIM**	**Dr**	**Univ. Of Sidi Bel-Abbés**

Program of The 3rd edition of the international conference on materials science and engineering and their impact on the environment -ICMSE'2024-

WEDNESDAY May 29, 2024 (Morning)			
08.00	Welcoming participants, distribution of documents and check in		
09.00 – 10.00	**Opening Ceremony**		
	A word from Pr AMERI Mohammed the President of the ICMSE 2024 Conference.		
	A word from Pr ATTOUCHE Mohammed Kadi The dean of the faculty of exact sciences		
	A word from Professor AMARNA Messaoud: Director of the Human Rights Laboratory at Algiers 3 University, Member of the National Economic, Social and Environmental Council and Secretary General of the National Federation of Higher Education and Scientific Research.		
	A word from Pr BOUZIANI Merahi the Rector of the Djillali Liabès University of Sidi Bel Abbès.		
10.00 – 11.00	 **Lecture 1 : Pr Aourag Hafid -** SMRIS-CRTI, Oran, Algérie **Pourquoi l'innovation en Science des Matériaux est très difficile ?.**		
11.00 – 12.00	**Coffee Break & Poster Session 1** **Evaluators:** **- Pr BOUKLI Hacen Amine** **- Dr BOUYAD Linda** **- Dr. SIDHOUM Mohammed**		
12.00 – 13.00	 **Lecture 2 : Pr JELLALI SALAH -** Sultan Qaboos University, Oman **Biomasses and mineral wastes turning into biochars : characterization and application for nutrients recovery from actual wastewater .**		
13.00 – 14.30	**Lunch**		
WEDNESDAY May 29, 2024 (Afternoon)			
14.30 – 15.30	 **Lecture 3 : Pr YARUB AL-DOURI -** Technology Innovation Institute, Abu Dhabi, United Arab Emirates **Future prespective of nanotechnology : Industial and biomedical application .**		
15.30 – 16.30	 **Lecture 4 : Pr Amar Tilmatin -** Univ. Of Sidi Bel-Abbés **Séparateurs électrostatiques des particules: application à la récupération des matériaux plastiques et métalliques .**		
14.40 – 16.00	**Oral Communications - Session 1 (Room A)** **Evaluators:** **- Pr BOUHAFS Bachir** **- Dr KHATIR Radja**	**Oral Communications - Session 2 (Room B)** **Evaluators:** **- Pr HARRACHE Djamila** **- Pr BOUYAKOUB Zahira**	**Oral Communications - Session 3 (Room C)** **Evaluators:** **- Dr. CHIALI CHARIF Khadidja** **- Dr. KHALDI Amina**

16.00 – 17.00		**Coffee Break & Poster Session 2** **Evaluators:** **- Pr BENZAIR Abdenour** **- Pr BENKHATOU Noureddine** **-Pr FASSI Benattou**	
16.20 – 18.20	**Oral Communications - Session 4 (Room A)** **Evaluators:** **- Pr RACHED Djamel** **- Pr BENKHATOU Noureddine**	**Oral Communications - Session 5 (Room B)** **Evaluators :** **- Pr HARRACHE Djamila** **- Pr BOUYAKOUB Zahira**	**Oral Communications - Session 6 (Room C)** **Evaluators :** **- Dr CHIALI CHARIF Khadidja** **- Dr. KHALDI Amina**

THURSDAY May 30, 2024 (Morning)

09.00 – 10.00		**Lecture 5 : Pr Hamrouni Bachir -** Faculty of Sciences of Tunis **Chemistry and materials science to cope with water scarcity.**
10.00 – 11.00		**Lecture 6 : Pr Samir Romdhane -** Tunis El Manar University, Tunisia **Organic Solar Cells : Material Innovations for a Sustainable Energy Future .**
11.00 – 12.00		**Lecture 7 : Pr MATTHEUS GOOSEN -** Alfaisal university, Saudi Arabia **Sustainable Development, Renewable Energy & Advanced Materials research .**

09.00 – 12.20	**Oral Communications - Session 7 (Room A)** **Evaluators:** **- Pr BOUHAFS** **- Pr BOUKLI Hacen Amine**	**Oral Communications – Session 8 (Room B)** **Evaluators :** **- Pr RAMDANI Nadia** **- Dr DRIZ Samia**	**Oral Communications - Session 9 (Room C)** **Evaluators :** **- Dr BOUYAD Linda** **- Pr BENGHAREZ Djamila**
12.00 – 13.00		**Coffee Break & Poster Session 3** **Evaluators:** **- Pr HIRECH HOUARI** **- Dr ARBOUCHE Omar** **- Dr TAYEBI Nadjia**	
13.00		**Check Out and Departure**	

Opening online communications

List of Oral Communications

14.40 – 16.00	**Oral Communications - Session 1 (Room A)**
14.40 – 15.00	**O-01 Abderrahmane Reggad** **Predictive properties of the nickel sulphide NiS**
15.00– 15.20	**O-10 Nehila Tarek** **Modeling and Simulation of Heat Transfer by Natural Convection with Periodic Heat Source in Fluid-Structure Interaction System**
15.20 – 15.40	**O-14 Tarik Ouahrani** **The role of intrinsic point defects on the production of green hydrogen fuel on the Cu2WS4 single-layer: ab initio calculation**
15.40 – 16.00	**O-23 mohand-amokrane lounis** **Structural Damage Identification in composite beam using modal data and metaheuristic**
14.40 – 16.00	**Oral Communications - Session 2 (Room B)**
14.40 – 15.00	**O-04 REZIG Naima** **Bending behavior of sandwich structures with glass and carbon fiber skin and PVC foam**
15.00– 15.20	**O-05 Merabti Mohammed Elamine** **Study of pharmaceutical products elimination by using carbon-based material**
15.20 – 15.40	**O-21 MITICHE LYNDA** **Transport sélectif des ions métalliques Cd(II) par D2EHPA dans une cellule microfluidique**
15.40 – 16.00	**O-25 FERHAT Mahmoud** **EXTRAITS DE PLANTES COMME INHIBITEURS DE CORROSION VERTS POUR LA PROTECTION DES METAUX**
14.40 – 16.00	**Oral Communications - Session 3 (Room C)**
14.40 – 15.00	**O-58 ALLAL Farida** **Green synthesis, characterization and antibacterial activity of eutectic mixtures of metronidazole**
15.00– 15.20	**O-59 charef mustapha abd el djabar** **Microbial fuel cell: a greener way to protect the environment**
15.20 – 15.40	**O-07 Manel Nardjes Toumi** **Impact of the Pulsed Electric Field on the extraction of the phenolic compounds of an industrial plant: Eucalyptus globulus**
15.40 – 16.00	**O-18 DEHAR Mokhtaria** **WATER TREATMENT WITH COMPOSITE BEADS (CALCIUM-ALGINATE/ACTIVATED CARBON)**
16.20 – 18.20	**Oral Communications - Session 4 (Room A)**
16.20 – 16.40	**O-19 Mohamed Amine Chenafi** **Impact of various doping elements on the structural and electronic properties of quaternary chalcogenides CZTS : DFT study**
16.40 – 17.00	**O-55 AMARI Malika** **Investigation of Structural and Magnetic Properties of Mn2ZrP: A Heusler Compound with X2YZ Formula**
17.00 – 17.20	**O-56 Houcine CHORFI** **Fine-tuning the strategy XtalOpt + Gibbs2 codes. Application to thermoelectric compounds (AgCl,**

	PbTe and CoSb 3) under stress: Phase diagrams pT
17.20– 17.40	O-02 ABDOUS Slimane Experimental Evaluation of Boron Carbide-Based Nanocomposite for Nuclear Shielding Against Highly Ionizing Radiations
17.40– 18.00	O-52 Khatir Radja First-principles investigation of: AgBr1−xIx (0 ≤ x ≤ 1) ternary alloys
18.00– 18.20	O-60 Ben Hamid Abdelkader International and National Efforts to Protect the Environment from Chemical Pollution Between Innovative and Traditional Mechanisms
16.20 – 18.20	**Oral Communications - Session 5 (Room B)**
16.20 – 16.40	O-33 BELKRALLADI HALIMA Traitements Plasmagéne et Plasmacatalytique D'un Colorant Anthraquinonique.
16.40– 17.00	O-08 loubna benhabib Optimisation of the photovoltaic efficiency of a cell based on GaAs
17.00 – 17.20	O-37 Wafà BENSTAALI Optimization of Sn2S3 BSF layer to imporove CIGS thin film solar cells
17.20– 17.40	O-42 BLAHA Lamia Farah Investigations of physical aspects of spinel AAl2O4 oxides via ab-initio calculations
17.40– 18.00	O-28 FASSI Benattou PbS Colloidal Quantum Dot-Based Photodetectors: A Promising Approach for Enhanced Performance in Visible Light Communication Systems
18.00– 18.20	O-47 TAYEBI Nadjia Investigation des propriétés structurales des nitrures de métaux de transition
16.20 – 18.20	**Oral Communications - Session 6 (Room C)**
16.40 – 17.00	O-06 Kheir Eddine KHODJA Cross-linked alginate biocomposite beads for Methylene Blue removal. Optimization study using a statistical approach based on a full factorial Design.
17.00 – 17.20	O-22 Fatima zohra ZEGGAI Highly Potent Antibacterial Copper-Based MOFs/Na-Alginate Composite Beads
17.20 – 17.40	O-03 BENADDA MOHAMED Terpolymer of Propylene Oxide - Styrene- Methyle Methacrylate
17.40– 18.00	O-27 DRIZ Samia Fiber Optic Nanotechnology: Shaping the Future of Communication
18.00– 18.20	O-24 AMERI Ibrahim Experimental study of structural inhomogeneities in Heusler materials
09.00 – 12.00	**Oral Communications - Session 7 (Room A)**
09.00 – 09.20	O-20 DENNAI Benmoussa Numerical Simulation of Tunnel Junction in Multi-Junction Solar Cells Using Silvaco Atlas Software.
09.20 – 09.40	O-36 Atouani Toufik Effect of the Electrodes Interface on Dye-Sensitised Solar Cell (DSSC) Performances
09.40 – 10.00	O-50 ZAZOUA Fatiha Ab initio full-potential study of properties and magnetic phase stability of rare earth diboride compounds
10.00 – 10.20	O-11 ABDELDJEBAR Hasnia THEORETICAL INVESTIGATION OF THE ANTI-ALZHEIMER POTENTIAL OF A NEW ORGANIC

	SUBSTANCE
10.20 – 10.40	**O-32 Hamza SOUALHI** **Influence of slag powder in rheological behavior of ecofriendly concrete**
10.40 – 11.00	**O-44 Abdallah Timmaoui** **Electrochemical characterization of the AMX anion exchange membrane in buffered solution.**
11.00 – 11.20	**O-57 Chafia Métaoui** **Magnetic, electronic, dielectric, Optic , Properties of emergent inverse Heusler metamaterial: Rh2HoSi**
11.20 – 11.40	**O-53 RACHEDI Samia** **Etude des propriétés physiques des matériaux piézoélectriques : premier principe de l'effet de la pression**
11.40 – 12.00	**O-16 Ramdani nadia** **Characterisation of leachates from the Sidi Bel Abbes landfill site and their treatment by adsorption on Hydroxyapatite**
09.00 – 12.00	**Oral Communications - Session 8 (Room B)**
09.00 – 09.20	**O-39 Chouikhi Manel Safia** **Elaboration of polymer network hydrogel for the removal of dyes from wastewater**
09.20 – 09.40	**O-40 Bachir ALLAM** **Optimizing thermal management and temperature control of building brick walls through integration of phase change materials: A case study in Bechar city**
09.40 – 10.00	**O-41 mekhloufi belkacem** **The impact of material choices on greenhouse gas emissions and climate change**
10.00 – 10.20	**O-45 Lina Benkraled** **Effect of Annealing and Plasticization on the Crystallization and Thermo-mechanical Properties of Poly(lactic acid)**
10.20 – 10.40	**O-48 Chaabane Lynda Amel** **The Determinants of PermeableConcreteBehavior:ExploringIntrinsicCharacteristics**
10.40 – 11.00	**O-31 Nour el houda BOUDA** **On the error analysis in NOMA networks: assessing the impact of environmental interference and imperfect SIC**
11.00 – 11.20	**O-12 CHIALI CHARIF KHADIDJA** **ESSAI D'ADSORPTION DU CADMIUM PAR UN CHARBON ACTIF ISSU D'UN DECHET AGROALIMENTAIRE**
11.20 – 11.40	**O-46 HAFFAF Wissem** **Synthesis and Characterization of Polymer-Based Nanocomposites Reinforced with Magnesium-Aluminum and Zinc-Aluminum Layered Double Hydroxides.**
11.40 – 12.00	**O-17 mahdjoub kheireddine zoubir** **Structural, electronic and optical properties of perovskites compounds XBS3 (X: Cs, In).**
09.00 – 12.20	**Oral Communications - Session 9 (Room C)**
09.00 – 09.20	**O-13 Ilyes BOULEDJOUAD** **Preparation and characterization of offertite zeolites exchanged with copper, silver, and zinc for antibacterial applications**
09.20 – 09.40	**O-15 Belmimoun Asmaa** **valorization of date seeds for the formulation of an activated carbon with a purifying effect on industrial oils**
09.40 – 10.00	**O-34 CHAHED HALIMA** **BaYAlZn3O7:Sm3+-based LEDs Leading the Way in Efficient and Sustainable Visible Light**

	Communication
10.00 – 10.20	O-35 KEBAILI RIMA Enhancing Next-Generation Optical Systems with PtSe2/ultrathin Al2O3/Ge -Based Photodetectors
10.20 – 10.40	O-51 Nabila AISSIOU Lignin-Phenylhydrazone as a Corrosion Inhibitor of API X52 Carbon Steel in 3.5%NaCl and 0.1 mol/L HCl Medium
10.40 – 11.00	O-38 Maroua Nihel BENABDALLAH Modeling for Electrical Conductivity of Polymer/Graphene Nanocomposites
11.00 – 11.20	O-54 Abd Elouahab Noua Enhanced photocatalytic activity of monometallic Ag, Cu nanoparticles loaded on ZnO prepared via modified polyol process
11.20 – 11.40	O-30 Hamza Medjadji Photocatalytic hydrogen production over MFe2O4 (M=Ca, Cu) nano-spinel powders under visible light irradiation.
11.40 – 12.00	O-29 Yerou Amine Mechanical Characterization of a biocomposite based on polypropylene reinforced with oyster shell particles
12.00 – 12.20	O-49 Rachid Ouhib Industrial Textile Wastewater Treatment And Potential Of Reuse

List of Poster Communications

Poster Session 1 29-05-2024 11.00 – 12.00		
P-001	Dra Rafik El Arslene	Adsorption of Methyl Orange and Methylene Blue by a Biomaterial: Kinetic and Thermodynamic Study
P-002	Benouali Mohamed Elamine	Synthe1 sis and application of nickel nano-composite
P-003	Ziani Zakaria Abdelhafid	Elastic, magnetic and electronic behaviors of EuFe4P12 Filled-Skutterudite: DFT+U study
P-004	Messadi Larbi	Elastic anisotropy and magnetic properties of CeNiSb Half-Heusler: First-principles investigation.
P-005	Khalida Mechttem	The Impact of Emulsifier on (1:1) Metronidazole:Ethylcellulose Nanoparticles' Characteristics
P-006	Benzaidi Orkia	Microporous Activated Carbon from wood waste and its Application in the Removal of Rhodamine B from Aqueous solution
P-007	Djebour Benali	Structural, elastic, electronic and dynamical properties of BaLiF3 Perovskite : Pseudopotentials study
P-008	Hanane Moussa	Structural and magnetic properties of PrCrO3 and PrVO3 magnetic perovskites: DFT+U study

P-009	**Mohammed Krarroubi Chaimaa**	Ab-initio study of new conventional superconducting materials
P-010	**Ouali Asmaa**	Modification and characterization of activated carbon using magnetic (Fe3O4) and ZnO nanoparticles
P-011	**Mohammed el amine Facih**	Advancements in Fuel-Rich Propellants: An In-depth Exploration of Boron Coreshell with Sodium Azide for Enhanced Combustion Efficiency in Propulsion Systems
P-012	**Louafi Elamine**	Spinel ferrite nanoparticles-graphene oxide nano-composite: synthesis and its catalytic effect on the thermal behaviour of nitrocellulose-based mixture
P-013	**Kalache Chaïmaâ**	Study of chemical composition and biological activity of differents plants
P-014	**Maiti Chaimaa**	Elaboration de Nanoparticules Mésoporeuses et Dégradation par Ozonolyse du Diclofenac de Sodium
P-015	**Mokrane Setti**	Study of structural and electronic properties of Perovskite SrMoO3 using FP-LAPW method
P-016	**Ait Amer Ahcene**	Preparation of a Novel Membrane of Poly (4-Chlorostyrene) clay composite, by cationic polymerization of p-Chlorostyrene using green catalysis
P-017	**Oussadi Karima**	Extraction of biopolymers from sheep's wool and their environmental preservation
P-018	**Khelil Mohamed**	Structural and optoelectronic of the triangular quaternary system BxIn1-xNyAs1-y
P-019	**Rahla Miloud**	matériaux composites à fibre végétale
P-020	**Sana Bakhta**	Prédiction des propriétés structurales , élastiques et électroniques de la pérovskite CaTaO3 .
P-021	**Belghoul Hafida**	Ab initio study of the structural, electronic and optical properties of BSb and BN compounds and their superlattices
P-022	**Zoubir Benkhanouche**	Simulation of the energy of graphene nanoribbons by the DFT method with the SIESTA code
P-023	**Benharat Samira**	Developing a novel model for replicating the electric discharge phenomenon in the rod-plane air gap system
P-024	**MEGHOUFEL Zahira Faiza**	High-efficiency thermoelectric converter material: First-principles calculations of KBiBa half-Heusler compound
P-025	**Rezig Walid**	Highly efficient removal of industrial dye under neutral conditions by UV photocatalysis process using novel TiO2/Fe diatomite composite
P-026	**Khatir Radja**	First-principles studies of novel lead-free halide double perovskite
P-027	**korichi hakim**	Study of the characteristics of the p+ emitters Produced during the metallization of the rear surface of n-type silicon solar cells
P-028	**Amina Dendane**	Optical and bonding properties of hybrid metal-halide (CH3NH3NP) PbX3 (X = Br) perovskite: A density-functional theory study
P-029	**Amine Abdelkader Guermoudi**	MEASUREMENT OF SILICON NITRIDE THIN-FILM THERMAL CONDUCTIVITY USING THE 3-OMEGA METHOD
P-030	**Abderrahmane Younes**	Magnetic and Structural Properties of FeTiO2 Nanocomposite Produced by Mechanosynthesis Technique
P-031	**Liamani Samira**	Contribution to the analysis of interfacial damage of biomaterials
P-032	**Nawal Belmiloud**	Structural, mechanical, thermodynamic and dynamic stabilities off NaCaN half-heusler compound
P-033	**Rachid Amraoui**	Impact of Cu on the Magnetic Properties of FeTiO2 Nanocomposite
P-034	**Oughreb Chewki**	Phonon and electronic transport properties of FeZrTe heusler alloy for thermoelectric applications
P-035	**Oumeria Khelladi**	Understanding the Mott Insulator to Superconductor Transition in Quasi-Two-Dimensional Iron-Based Compounds: A Density Functional Theory Study
P-036	**Drici lamia**	The structural, elastic, electronic and optical properties of CaCuP and CaAgP alloys have been investigated through first-principles calculations.
P-037	**Merah Somia**	Study of the physical properties of halogen-based perovskite materials

P-038	**Nebbat El Amine**	On Vortices structures in non ideal magnetized dusty plasma
P-039	**Bouam Newres**	Planning the Trajectory of a Mobile Robot Using the A(*) Star Algorithm
P-040	**Nardjes Randa Hamdaoui**	Influence of Ag doping on opto-electrical properties of copper oxide thin layer deposited by spray pyrolysis root
P-041	**Mohamed Kouider Amar**	Predictive Modeling of Intrinsic Viscosities in Polymer Solutions Using Advanced Algorithms
P-042	**Fatma Riahi**	Structural and photoluminescence properties of Li co- doped (GdxLu1-x)2O3: 5% Eu3+ nanomaterials scintillators prepared by sol gel method
P-043	**Malika Saidi**	Elaboration et caractérisation de composites à matrice polyuréthane nanochargée avec des nanoparticules de ZnO-La
P-044	**Rachida Douani**	Elaboration de détecteurs d'humidité à base de biocomposites kératine/ x% nanoparticules d'argent.
P-045	**Mazari Halima**	Optimisation of a heterojunction solar cell: InGaN/SnS
P-046	**Amel Dadda Khorsi**	Analysis of radioactive materials behavior in the environment during the nuclear accident
P-047	**Cheridi Amina Lyria**	Numerical study of the ambient temperature influence on a vortex tower performance
P-048	**Mounir Ould-Mohamed**	Theoretical Prediction of Monolayer ScHfNO2 as a Potential Material for Ultraviolet Photodetection
P-049	**Ahmed Chabane**	Multi-Objective Optimization of Biodegradable Polymer-Based Microspheres Loaded with Candesartan Cilexetil
P-050	**Merazi Sayah**	The amplitude distribution of the total enthalpy flux at the cathode interface in TIG welding
P-051	**Kheira Ameur**	Predictive Study and Simulation of the Photoelectric Behavior of a CH3NH3PbI3 Perovskite Solar Cell
P-052	**Belgacem Leila**	Effect of shielding gas on tungsten cathode performance during DC TIG welding
P-053	**Arbouz imene**	Adsorption and degradation of methylene blue (MB) Dye Using nonlinear optical (NLO) active copolymer composite
P-054	**Brahim Guezzen**	Analysis of adsorption of Congo red dye onto trioctylmethylammonium modified Algerian bentonite using Box-Behnken design approch
P-055	**Mekhalef Benhafsa Leila**	Ab-initio study of TlGeX3 (X= Br, Cl) for photovoltaic applications
P-056	**Lounis Zakia**	Stability Analysis of SnO2 Thin Film Gas Sensors Using tools (AES, EELS and AFM)
P-057	**Douma Bouthiba Asma**	Structural, Electronic, and Elastic Properties of New Halid Peroveskite (RbRaI3) from Ab initio Calculation.
P-058	**Amel Mekki**	Catalytic behavior and antibacterial/antifungal activities of new MNPs/zeolite@ alginate composite beads
P-059	**Meryem Romaissa Djellouli**	Inter-Satellite Simulation with Custom Modulation: Enabling DVB-RCS2 Integration with Optical Communication Networks
P-060	**Amira Delloum**	Investigating the Structural and Electronic Properties of AlN/GaN Superlattices Along (110), (110), and (111) Growth Axes Using First Principles
P-061	**Khatir Ouail**	Theoretical investigation of structural, mechanical, and thermodynamic properties of HfX2 (X=S, Se) using first-principles calculations
P-062	**Bouaziz Ilhem**	Multilayer Perceptron using Molecular Descriptors to model the Essential Oil Yield from Medicinal Herbs
P-063	**Mehdi Hammar**	Exploring Green Solvents for the Separation of Imidacloprid from Aqueous Environments: A Theoretical Study on Behavior, Stability, and Environmental Implications
P-064	**Noreya Bestaoui-Berrekhchi Berrahma**	Exploring the Structural, Electronic Properties and Reactivity of Benzimidazole derivative in Solvent Environment using DFT Study
P-065	**Bouam Abdallah**	Influence Analysis of the Ambient Conditions on the Vortex Tower Prototype Performance
P-066	**Bellahcene Fatima Zohra**	Ab-initio invstigation of structural,electronic, magnetic and optical proprieties

	Zoulikha	of a novel double perovskite : Sr2CeRuO6
P-067	**MEDJDOUB Lahouaria**	Synthèse d'un matériau hybride-Organophosphazène- catalysée par l'argile(MaghniteH+)
P-068	**Ghribi Saadia**	The internal repair by bonding the composite patch
P-069	**Moufida Beroual**	Physicochemical properties of nanocrystalline cellulose isolated from artichoke microcrystalline cellulose
P-070	**Dahia Ahmed**	Source term calculation and risk evaluation during accidental release of BWR Nuclear Reactor
P-071	**Boussahra Sarra Mama Nor El Houda**	Étude numérique du facteur d'intensité de contrainte dans les structures navales endommagées par fissuration
P-072	**Marwa Jdidi**	Adsorption of cationic dyes using surfactant modified algerian clay : kinetic and adsorption mechanism studies.
P-073	**Badi Ridha**	Numerical Simulation of The Mechanical Behavior and Feasibility of a Hip Prosthesis Architecture.
P-074	**Rebiha Bencherik**	Reinforcement of the properties of biodegradable PLA-based films by integration of nanoparticles and bioactive agent
P-075	**Douaa Khelladi**	Homogenization of Heterogeneous Structures Using the Finite Element Method
P-076	**Redjouh Nour Elhouda**	Deposition and Characterization of Nanostructured Copper Oxide (CuO) Thin Films using Sol-Gel Dip-Coating Technique
P-077	**Abderahim Abada**	Magnetic and structural properties of nanostructured FeSn alloys elaborated via ball milling process
P-078	**Boukais Meriem**	Effect Of The Absorbent Layers On The Performances OF The SiGe Thin-Films Solar Cell
P-079	**Lemya Amrani**	Ab-initio calculations of structural ,electronic,optical and thermoelectric properties of a noval hybrid double perovskite Na2LiMgH6 compound for advanced energy storage system
P-080	**Abdelli Abdelbasset**	Computational prediction of structural, electronic, elastic, optical and thermoelectric properties of YVReZ (Z =Al , Ga, In) Yttrium based quaternary Heusler alloys for optoelectronic and thermoelectric applications: A DFT study.
P-081	**Talbi Khedija**	Electronic and thermoelectric properties of Half-Heusler compound: Spin orbit coupling effect
P-082	**Aidrous Hakima**	Effect of Magnesium on the dielectric properties of an alloy (Al-3%Mg) alloy for humidity sensor applications
P-083	**Alili Nabila**	Impact of Convergent Angle Variations on Rocket Nozzle Performance parameters
P-084	**OUAHAB Iman**	All Optical 1D Ternary Photonic Crystal Biosensor for Detection of Cancerous Brain cells
P-085	**Dine el hannani mohamed**	First principle investigation of structural, electronic and magnetic properties of cubic LaFrO3
P-086	**Mme. Boukertouta Ghadir**	Investigation Of Re(I)-Tricarbonyl 1-2-4 Triazol Complexes By DFT Method
P-087	**Mohammed Amine Djeffal**	Numerical Investigation of Aspect Ratio Impact on Regenerative Cooling Heat Transfer in Liquid Propellant Rocket Engines
P-088	**Amel Slamani**	Investigation of structural, mechanical, electronic and thermodynamic properties of YLuNi2Sb2 double half Heusler: FP-LAPW Method
P-089	**Guermit Youcef**	Revealing half metallicity of new full-Heusler compound
P-090	**Hocine Kamel**	A computation exploration of physics properties of new iradium based fulHeusler
P-091	**Labdelli Boutaleb**	Effects of oxygen flow during the annealing process of doped emitters in n-type monocrystalline silicon wafers.
P-092	**Rebehi kheira**	Study of the Mechanical Behavior of a Standardized Arc-shaped Specimen in PVC
P-093	**Bassou Djilali**	Synthesis , characterization and bio activities of poly(1-2(Dihydroxyethyl)-3-vinylimidazolium) (poly (ionic liquids))

P-094	**Leila Djazia Benmansour**	Wave propagation response of double – walled carbon nanotubes
P-095	**Zakia Fekih**	Optimization of experimental parameters for the electrodeposition of Cobalt-Molybdenum metal layers on a silicon substrat
P-096	**Ouari Kheira**	Investigating Thin Films of Lead Sulfide (CdS): Production, Analysis, and Theoretical Perspectives for Implementing Biological Detection Devices.
P-097	**Miloudi Mohamed Esseddik**	Structural, electronic, elastic and optical properties of Sc based equiatomic quaternary Heusler compounds
P-098	**Iles Amel**	Classical and ultrasonic preparation of new copper based nanocomposites: Application in the antimicrobial activity
P-099	**Mr. Zehouani Mohammed Aymen**	moleculary imprinted films for bisphénol A retention
P-100	**Blaha Nesrine Hadjer**	Enhancement in Photocatalytic Properties of Sn-Doped La2O3 Nanostructures
P-101	**Debboub Salima**	Study of the antimicrobial effectiveness for spinel ferrite nanoparticles of manganese-cobalt doped with cerium
P-102	**Zouheyr Dif**	Comparative study of ground-motions predicted using stochastic and neuro-fuzzy models
P-103	**Megherbi Radja**	Vers de Nouveaux Horizons: Nanocomposites d'Argent à Base de Copolymères Greffés Intelligents PVA-g- (PAA co PS)
P-104	**Nour el houda Bouda**	Non-Orthogonal Multiple Access for Enhanced Cellular Vehicle-to-Everything Communication
P-105	**Benaichouba Zahira**	Comparative Evaluation of Mechanical Properties of Virgin and Recycled Polypropylene after Aging
P-106	**Chellali Abdelhamid**	Structural, electronic and magnetic properties of inverse-Heusler alloys Mn2ZrGe: A first-principles investigation.
P-107	**Zeggai Nadjet**	Structural &Magnetic Properties of DMS
P-108	**Blaha Lamia Farah**	Structural , electronic and thermoelectric properties of antiperovskite compound Sr3SiO : A first principles study
P-109	**Benhadda Abir**	Marine Algae-Derived Activated Carbon: A Sustainable Solution for Pollutant Removal.
P-110	**Berrouna Henen**	Ab-initio predictions of Structural, electronic and magnetic properties of double-Ge-layer MAX phase Cr2Ge2C
P-111	**Abderrahmani Fouzia**	Synthesis and characterization of CeNiO3 Perovskites to Nitrophenol degradtion
P-112	**Mohammed Cherif Terkhi**	Green synthesis of ZnO nanoparticles from castor oil leaf extract: Environmental use, kinetic and thermodynamic studies of adsorption of a toxic dye.
P-113	**Benyettou Mohammed**	Analysis of the effect of aging duration in water immersion of a damaged structure repaired by the bonding process.
P-114	**Abdelkrim Benarroudj**	Comprehensive Analysis of the Structural, Electronic, Elastic Properties of ternary chalcogenides pnictogens InPnS3 (Pn=Bi, Sb) Compounds: First-Principles Calculations
P-115	**Izzeddine Allali**	A Robust Interval Type-2 Fuzzy Logic Controller of a Doubly Fed Induction Generator for Wind Energy Conversion
P-116	**Semane Rabea**	Activation of persulfate by several methods to degrade polyphenols contained in olive mill waste water
P-117	**Hamamouche Kahina**	Effect of Ultrasound, Microwave Assisted Extraction On Seaweeds Material
P-118	**Boutarfa Hayette**	Electrochemical studies of anodic oxide films on titanium and TA6V alloy.
P-119	**Ibrir Abdellah**	Modeling of Drug-Protein Binding Fraction (FB) by CNN-MLP
P-120	**kheirallah mohammed**	Ab initio electronic structure and magnetism in Sr2MOsO6 (M= Cu or Ni) double perovskite systems: a GGA+U and GGA + U +SOC
P-121	**Drief Mohammed**	Half-metallic ferrimagnetic characteristics of Ti2-based ternary Heusler alloys.
P-122	**Bouragba Djamel**	Effects of nitrogen incorporation on the optoelectronic properties of BSb binary compound: Optoelectronic application

P-123	**Habeche Fatima**	Mesoporous silica doped with AgNPs/CeO2 nanoparticles for water pollutant reduction.
P-124	**Zahraoui Mehdi**	New method of valorization of natural materials and their applications.
P-125	**Cherifi Wafa Nor El Houda**	PREDICTION OF CORROSION POTENTIAL USING THE GENERALIZED ARTIFICIAL NEURAL NETWORKS METHOD
P-126	**Sehoul Baghdad**	FIRST PRINCIPLES CALCULATIONS TO INVESTIGATE STRUCTURAL, ELECTRONIC AND THERMOELECTRIC PROPERTIES OF LiZnP HALF-HEUSLER
P-127	**Debboub Salima**	Influence of various heat treatments on elastic parameters of CuZnAl shape memory alloy
P-128	**Ouafia Liamani**	Antimicrobial activity of mint essential oils
P-129	**Cherifa Hakima Memou**	ADSORPTION OF PARA-NITROPHENOL ON CYCLODEXTRIN BASED-MATERIAL COATED BY BENTONITE
P-130	**Hakim Bouzemlal**	Adsorption Modeling of Various Phenols on Activated Carbon Fibers using Convolutional Neural Network (CNN) and Support Vector Machine with Dragonfly Algorithm
P-131	**Mohammed El Amine Boulekbache**	Electronic and optical properties of Hg1-xCd xTe ternary alloys
P-132	**AMERI Mohammed**	Structural, elastic, thermodynamic and electronic properties of LuX (X = N, Bi and Sb) compounds: first principles calculations
P-133	**Belhadji KinzaAmel**	Biosynthèse de nanoparticules de ZnO et évaluation de leurs propriétés chimiques et biologiques.
P-134	**Halima Delali**	Isotherme d'adsorption d'un colorant cationique par charbon actif à base de coques de noix
P-135	**Bourahla Asma**	First Principale calculations of structural,elastic,électronic and magnetic propretiesofAg2BGd fullHeusleralloycomoundsusingGGAandGGA+U: FP-LMTO calculations
P-136	**Manal Chettibi**	Molecular docking and pharmacokinetics studies of a synthesized Schiff base
P-137	**Chinoune Kheira**	Application of the sorption process in the elimination of MB in aqueous solution by Alginate-sepiolite biocomposite beads: adsorption kinetic, and modeling
P-138	**Ghalem Ikram**	Solubility of asphaltenes in two polar solvents
P-139	**Kandouci Chahinaz**	O-LiDAR performance analysis for different Jerlov water types
P-140	**Amer Mecellem**	Numerical analysis of residual stresses and warpage of thin-film coated silicon wafers
P-141	**El Badaoui Naima**	Physicochemical and biological characterization of residual discharges from the National Electronic Industries Company of Sidi Bel Abbes and risk assessment.
P-142	**Lilia Beldi**	Ab-initio Investigation of the Structural and Dynamical Stability of Ni2MnSi Full-Heusler Alloy.
P-143	**Dellali Mohammed**	Development of microparticles based of polysaccharides as novel drug release systems
P-144	**Saadia Belkiour**	Preparation of a new composite by ultrasonic method(catalytic reduction application)
P-145	**Safa Abdelkader**	Thermal vibration analysis of FGM Structures
P-146	**Fatma Remil**	The mechanical behavior of polymer biomaterials
P-147	**Nadir Hachemi**	Microscopic study of the effect of desert environmental factors on the materials that make up solar panels .
P-148	**Boumendil Sonia**	Comparative study of the environment in metal complexes. DFT and TD-DFT study
P-149	**Meftah Souad**	Optimization of Tin Bath Parameters to Enhance Efficiency in 3mm Thin Glass Production
P-150	**Abdelkarim Brahimi**	Optimization of adsorption capacity: Application of mathematical modeling
P-151	**Saadaoui Fatiha**	Structural, elastic, electronic, and optic study of the anti-perovskite Rb3BrO
P-152	**Djeffal Rachid**	Le rôle efficace des matériaux à changement de phase (MCPs) dans la résolution de problèmes thermiques anciens *Résumé d'une étude approfondie*

P-153	**Dhilal Alouani**	Simulation Study of Semiconductor Perovskite CsGeCl3 for Future Solar Cells Applications
P-154	**Belkassam Yamina**	Differential immunochemical characterization of monoclonal antibody directed against the beta-casein and its proteolysis products by the plasmin
P-155	**Hellal Tijania**	BIBLIOGRAPHIC REVIEW ON THE VARIOUS METHODS AND TECHNIQUES OF PHYTOTECHNOLOGY
P-156	**Mohammed Cherif Ramdani**	Optimizing Performance of Perovskite Solar Cells Based on triple cation Perovskite solar cell through SCAPS-1D Device Simulation
P-157	**Benaissa Wissem**	Simulation study of chalcogenide perovskite (BaZrS3) solar cell by SCAPS-1D
P-158	**Ghribi Saadia**	Finite element analysis of repair of composite laminates by bonding External patch
P-159	**Amel Benmansour**	Monte Carlo study of the multilayer system and magnetic properties of the Site-disordered Blume Capel model.
P-160	**Hayat Tati**	Composite pipelines susceptible to Hydrogen embrittlement : new proposal technics on the protection methods
P-161	**Hocine Hayat**	A density functional theory study of the thermoelectric properties of CuMg2InS4
P-162	**Fatima BEKKAR**	Synthesis and characterization of a new chelating foaming phenolic resin for extraction of rare earths elements
P-163	**Fatma Larbi**	Etude de l'effet de l'incorporation de nanocristaux et de nanofibres de chitine sur la structure et propriétés de l'hydroxypropyl méthylcellulose (HPMC)
P-164	**Kheira Hamaida**	A first-principles investigation of the structural, mechanical, electrical, and optical characteristics of a novel quaternary SrFZnAs compoundMechanical, electrical, optical, and structural characteristics of a novel quaternary SrFZnAs compound: An understanding from the ground up
P-166	**TAYEBI Nadjia**	Structures électroniques et propriétés magnétiques des nitrures de métaux de transition
P-167	**Chaabane Lynda Amel**	LES ENJEUX DU BETON DRAINANT PAR LA METHODE DE DREUX GORISSE
P-168	**Bouyakoub Amel Zahira**	Treatment of Textile Effluents by Combined Methods
P-169	**Rachid Ouhib**	Removal Of Azo-Dye From Synthetic Wastewater By Coagulation
P-170	**Belkhouane Samira**	Etude des propriétés structurales, électroniques et thermodynamiques d'un alliage quaternaires Cu2CdSnS4 par la méthode du potentiel total-linéaire des orbitales muffin-tin (FP-LMTO)
P-171	**Badaoui Asmaa**	Synthesis and characterisation of triple-reponsive copolymer hydrogels based on 2-(dimethylamino)ethyl methacrylate and acrylic acid : an intelligent materials chemically cross-linked developed for treatment and dyes removal
P-172	**Lazreg Hadji**	Free vibration analysis of porous multi-directional FG sandwich plates
P-173	**Souad Benkherbache**	Numerical Simulation of heat transfer of hybrid nanofluid In PV/T solar panel
P-174	**Guermit Mohamed Bilal Chami**	Free vibration analysis of FG sandwich beams with porosity
P-175	**Latreche Laid**	Effect of swap defect on the electronic and magnetic properties of quaternary heuslers alloys
P-176	**Bendaida Mohamed**	Analyse Dynamique des nano-structures en FGM
P-177	**Ameri Ibrahim**	Study of the spin collapse in orthoferrite using LDA+U
P-178	**Belkralladi Halima**	Identifiquation d'une plante endimique de la region Sud ouest algerien.
P-179	**Meryem Mouffok**	Influence of Polymer Types and Concentrations on Losartan Controlled Release Microparticles
P-180	**Ghali Drici**	THE WINKLER FOUNDATION STIFFNESS EFFECT ON THE VIBRATION CHARACTERISTICS OF FGM NANO-BEAM USING THE FINITE ELEMENT METHOD
P-181	**Baira Fayçal**	Deformation and Electronic Properties of Amorphous Tubes under the Influence of Electric Fields
P-182	**Moulay Awatif Amaria**	REUSE WASTEWATER
P-183	**Maoudj Hanane**	Prediction of materials with high thermoelectric efficiency at high pressure.

P-184	**Hanagria charifa chahrazed**	Synthèse et caractérisation des composites magnétiques et modification par différents concentrations de Ctab pour l'adsorption des terres rares
P-185	**Chekroun Mohamed Zoheir**	Experimental and numerical study of ZnO nanoparticles
P-186	**Toufik Mana**	Wear behavior of copper alloys thermal spray coating
P-187	**Djefal Abdelkader**	Study of the electronic and magnetic properties of the double perovskite Ca2CoMoO6
P-188	**Hachilif Asma**	A Theoretical Study Of A Dynamical Stability of A Novel Double Spinel Zinc Ferrite.
P-189	**Harmel Meriem**	First principles study of the double perovskite compound Ba2RhWO6 for optoelectronic applications
P-190	**Mahdjoub kheireddine zoubir**	CrYSi (Y= Be, Ra), a half-Heusler with half-metallic ferromagnetic properties: a DFT calculation.
P-191	**keniche Assia**	Removal of Copper from Industrial Wastewater by seeds of Moringa
P-192	**Smain Mesbah**	Investigation of A2AlAgCl6 (A=Rb, Cs) using first principles: Potential utilization in UV optoelectronics
P-193	**Mohammed Houari**	Exploring the Physical and Optoelectronic Properties of Co2ZrZ Compounds: Insights from Computational Analysis and Thermoelectric Characterization
P-194	**Izzeddine Allali**	Commande hybride glissant flou d'un système éolien à base d'une génératrice asynchrone à double alimentation

List of Online Communications

01-06-2024 14h00-17h00	**Online Session 1 Evaluators: - Dr BOUYAD Linda -Dr BLAHA Lamia Farah**	
ON-001	**Charif Rania**	CASTEP investigation of structural, electronic, and optical properties of NiSb2O6
ON-002	**Djedjiga Ben Abdesselam**	L'influence du glucose sur le dépôt d'argent et la résistance à la corrosion de l'acier inoxydable austénitique 316.
ON-003	**Chenoui Mohamed**	zero-dimensional Modeling of Dielectric Barrier Discharge in Pure Carbon Dioxide.
ON-004	**boulahia salma**	E-pharmacophore modelling, virtual screening studies and in-silico ADME analysis for identify new anticancer compounds
ON-005	**Boucif Fatima**	Removal of Indigo Carmine by Mg/Al layered double hydroxide
ON-006	**Bensaci Zineb**	The use of solar photovoltaic energy in the field of water treatment
ON-007	**Belgharri Benali**	Synthesis of FePO4 modify by Nickel, and their application in organic synthesis
ON-008	**Attouti Salima**	Prédiction de l'isotherme d'adsorption optimale : Comparaison des modèles linéaires et non linéaires
ON-009	**Ayadi Souad**	Wear Behavior of Nb-V-Cr Alloyed High Manganese Steel
ON-010	**Amel Gasmallah**	Study of the properties of selenium monochalcogenides SnSe and ZnSe by ab-initio simulation
ON-011	**Belhamideche Kheira**	Efficiency of a shallow geothermal heat exchanger with soil-atmosphere interaction for space heating and cooling in the city of Mostaganem.
ON-012	**Wissem Gouasmia**	Physical properties of Silver Gallium Telluride (AgGaTe2) for sustainable energy technologies applications: A Density Functional Theory Study
ON-013	**Asma Bahloul**	synthèse et application des nanoparticules

ON-014	**Bendellaa Ramila Chahinez**	Biosorption of an inorganic pollutant from aqueous solutions
ON-015	**Boumaiza Abdelaziz**	Effect of the Magnetic Field on Heat Transfer in a Corrugated Channel
ON-016	**Terkhi Sabria**	Thermodynamic and Thermoelectric Properties of Ternary Half-Heusler Alloy: Suitable for green energy applications
ON-017	**Yasmine Cheddani**	Synthesis and characterization of rare earth based coordination polymers with succinic acid and 1,10-phenanthroline
ON-018	**Sonia Chebouki**	Investigating RbMgH3 Perovskite as Promising Material for Future Hydrogen Storage.
ON-019	**Maoudj Hanane**	Prediction of materials with high thermoelectric efficiency at high pressure
ON-020	**Omar Elfarouk Houache**	Cocrystal Formation of the API Captopril with L-Arginine and L-Proline: Experimental and Theoretical Insights with DFT Analysis
01-06-2024 14h00-17h00		**Online Session 2 Evaluators: - Dr MESBAH Ismail - Dr Kandouci Chahinaz**
ON-021	**Mounia Alayat**	AB-initio study of the structural, electronic and optical properties of AlN and AlBi binary compounds by the Wien2k code
ON-022	**Hemza Mancer**	Ab initio investigations of the structure-stability, electronic, and magnetic properties of Cr-doped Na2S
ON-023	**Sadou Mohammed**	Elaboration and Characterisation of Mesoporous Materials. Study of Catalytic Properties.
ON-024	**Briki Hayet**	Synthèse et Hydrolyse du polyacrylamide. Effet de la complexation par les ions bivalents.
ON-025	**Mohamed El Amine Khiari**	Predicting Damage in CFRP Bi-Graded Plates with Glass-Epoxy Materials
ON-026	**Abdelkader Benkhettou**	Optimization of a customized passive polyurethane foam mattress to optimize the human body's sleeping position
ON-027	**Youcef Daoudi**	Ab intio investigation of electronic and magnetic properties of Ca1-x TMx Te (TM= V, Cr, and Mn).
ON-028	**Mohamed Esseddik Ouardi**	Conception of SPR-based sensor for cancer cell detection
ON-029	**Fatna Telli**	Using FGM to Predict Damage in carbon-Epoxy Composite
ON-030	**Mekersi Romaissa**	Synthesis, characterization of the perovskite Eu-doped KNbO3 and its application for hydrogen evolution under visible light
ON-031	**Bendahah Abla**	Study Of The Physical Properties Of Binary And Ternary Compounds Based On Samarium (Sm)
ON-032	**Hemza Mancer**	the effect of different exchange-correlation functionals on the electronic structure properties of chalcogenide compound Ag2Se
ON-033	**Chadi Kamel**	The effect of mini channel geometries of AlSi10mg aluminum alloy cooler on the flow and thermal characteristics
ON-034	**Asli Faiza**	Docking Moléculaire et Pharmacocinétique Appliqués à Une Série D'hétérocycles Quinazoline et Quinoléine
ON-035	**Yasmina Bouleghebar**	Properties of Self-Compacting Mortar Containing Glass and Brick Powder
ON-036	**Saidani Abdelmadjid**	Molecular modulation of Falcarinol in Anethum graveolens herbal essential oil against anti-inflammatory activity
ON-037	**Blizak Meriem Djanette**	Synthesis of NiO nanoparticles by the Pechini sol-gel method
ON-038	**Naima Mekhloufi**	An experimental study to improve the efficiency of the solar still by adding stuffed tubes to the still basin
ON-039	**Melaab Loubna**	Well Thickness Dependent Rashba Parameter and Spin Splitting in a (100) Grown GaAs/AlGaAs Double Quantum Well
ON-040	**Benchaib Nadia**	Numerical investigated to predict the damage in composite beam under tensile load

02-06-2024 14h00-17h00	Online Session 3 Evaluators: - Dr BOUYAD Linda - Dr MESBAH Ismail	
ON-041	Zohra Bouchekhou	Development and Characterization of a Ternary Inclusion Complex for Improved Niflumic Acid Delivery
ON-042	Smati Sabrina	Density functional theory and molecular docking study of a novel organic pyrrole-based material
ON-043	Nesrine Labdouni	Numerical Study of Ozone Generated by Dielectric Barrier Discharge in O2-Ar Mixture
ON-044	Fekkar Nadia	DYNAMIC BEHAVIOUR OF CONFINED N-HEPTANE AND WATER IN BIFUNCTIONALIZED MESOPOROUS ORGANOSILICA SBA-15
ON-045	Mansour Houda	A Density Functional Theory Exploration of InAs/GaSb Superlattices for Optoelectronic Potential
ON-046	Amina Lahouali Dit Yahyaoui	2-thioxo -3N-(2-ethoxyphenyl) -5[40-methyl -30N-(20-ethoxyphenyl) thiazol-20(30H)-ylidene] thiazolidin-4-one: Growth, spectroscopic behavior, single- crystal investigation, Hirshfeld surface analysis, DFT/TD-DF computational studies and NLO evaluation
ON-047	Massillia Ait Radi	Ultrasound-promoted Elaboration of Novel Nanocomposites Based On a New Semiconducting Copolymer and Magnetite Nanoparticles Fe3O4: Application in Anionic Dye Adsorption
ON-048	Meddah Araibi Nourredine	Study of The Inhibitory Efficiency on a Steel of Type API 5L X52
ON-049	Imane Bensahbane	COMPUTATIONAL STUDY OF NEW PHTALIMIDO 1, 3-THIAZOLE DERIVATIVES AS CYTOTOXIC AGENTS FOR LEUKEMIA DISEASE
ON-050	Belacheheb Wafaa	The influence of green solvent on the synthèses yield
ON-051	Benssassi Mohamed El Hadi	Bismuth Ferrite as an efficient heterogeneous photo-Fenton-like catalyst for remediation of water contamination
ON-052	Rafik Marir	Evaluation of a Novel Polymer as a Bio-Coagulant for Fruit Juice Wastewater Treatment
ON-053	Belkacem Fatima Zohra	Optimization of pesticide adsorption conditions by intercalated halloysite: equilibrium isotherm study and modeling.
ON-054	Boudjellal Djamel	Valorization of vegetal biomass based lignin
ON-055	Chebahi Asma	Eco-Friendly Synthesis of Biodegradable Plastics : A Study on PHB Production Using Locally Isolated Bacillus sp.
ON-056	Boughanem Mohd Oulmessaoud	Elaboration and characterization of pure CuO, pure ZnO, and ZnO/CuO nanocomposite.
ON-057	Benouadah Nacera	Valorization of Eucalyptus camaldulensis inner and outer barks for biopolymer applications
ON-058	Guettai Hakima	Synthesis of nanotubes based on tartaric acid
02-06-2024 14h00-17h00	Online Session 4 Evaluators: - Dr KHATIR Radja - Dr BLAHA Lamia Farah	
ON-059	Benarbia Meriem	Elaboration de poudres de phosphore Lux Gd1-xPO4 dopées au Pr3+ par méthode sol gel
ON-060	Bouabida nour El houda	Synthesis and characterization of Nanocomposite of aniline and 2-chloroaniline by polymerization in-situ
ON-061	Kazi Tani Mohammed Yacine	Fabricate a triboelectric nanogenerator from SnO2 co-doping fluorine and aluminum
ON-062	Ouardia Zekri	Facile Preparation of a Supported Copper-modified HMS.
ON-063	Messas Amar	Empirical model for masonry infill under lateral loading through extensive database

ON-064	**Naamoun karima**	Adsorption of asphaltenes in presence of nanoparticules
ON-065	**Hafida Zerigui**	Synthesis of superabsorbent biopolymer and its applications
ON-066	**Khettar Amina**	Simulation of a Vehicle Suspension System Using two Control Strategies
ON-067	**Makhlouf Fatima Zahra**	Nickel nanoparticles-decorated graphite-modified screen printed electrode toward the electrochemical determination of dopamine
ON-068	**abboud abir**	Experimental Investigation on Improving Refrigeration Systems Performance Using Phase Change Material
ON-069	**Guerfi Meriem**	Novel α-sulfamidophosphonates analogues of Fotemustine: Efficient synthesis using ultrasound under solvent-free conditions
ON-070	**Sefiane Naima**	Effect of Gd3+ incorporation on structural and luminescence properties YAG phosphors powder doped with Ce3+ synthesized by sol-gel method
ON-071	**Chami Sabah**	Effect of temperature and pressure on the thermodynamic properties of Fe2-xNiGa1+x Heusler alloys: An ab initio study
ON-072	**Djouher Addadj**	Study of the Anti-corrosion Properties of an Expired Drug for Steel in Hydrochloric Acid: Environmental Protection
ON-073	**Boukebbous Ines**	ÉVALUATION DE L'EFFICACITÉ DE L'HYDROXYDE DOUBLE LAMELLAIRE Mg-Fe POUR L'ÉLIMINATION DU BORE EN PESENCE DES IONS COMPÉTITEURS
ON-074	**Sarra Harkati**	Improved Mechanically Alloyed Fe-Mo-P Powders Properties for Industrial Exploitation
03-06-2024 14h00-17h00		**Online Session 5 Evaluators: - Dr BOUYAD Linda - Dr BLAHA Lamia Farah**
ON-075	**Radja Nour El Imene Bennoui**	Half-metallicity from NaVAs half-Heusler alloy with stable structure in ferromagnetic state
ON-076	**Benyakhou sarah**	Préparation et caractérisation de matériau hybride à base de poly-2 Aminophényl disulfide renforcé par Silica Gel
ON-077	**Louati Nesrine**	Ab-initio Study of Structural, Electronic And Optical Properties Of AgAlTe 2 Compound in the framework of DFT
ON-078	**Barkat Lamia**	Elaboration and Characterization of Copper-doped tin Oxide Thin films for Photovoltaic applications
ON-079	**Oussama DRICI**	DFT Calculation of the Structural, electronic and optical properties of the chalcopyrite compound MgSiP 2
ON-080	**Amar Anissa**	Influence of Charge Transfers on two-Photon absorption cooperative effects within multi-Dipolar Ruthenium Complexes
ON-081	**Afoun Meryem**	Absorption of méthylène blue dye from a liquid solution using an organométallic matériel based on iron nitrate
ON-082	**Hamadi Zineb**	Application of Heusler Materials in the Reduction of Greenhouse Gas Emissions
ON-083	**rim roukya Belhoula**	Electronic and optical properties of strained Al1-xGaxN
ON-084	**Sadaoui Loubna**	Removal of heavy metals by valorization of agricultural biochar: effect of different activator solutions.
ON-085	**Horiya Benharchache**	The Impact of Exterior Walls on Algerian Rural Buildings' Energy Efficiency in Various Climate Zones
ON-086	**Mechenene Mohamed Lamine**	A comprehensive analysis and identification of Lemaitre damage model parameters of DC04 metal sheet.
ON-087	**Charif Majda**	Doped Bio-Calcium with semi-condicter (Aurivillius) for the Dégradation and élimination of organic polluants
ON-088	**Zanoune Kheira**	Polymeric Nanocapsules Loaded with 5-Fluorouracil for Targeted Cancer Therapy
ON-089	**Badiaa Bachiri**	Optimizing Performance of KSnI 3 -Based Perovskite Solar Cells with Tin (Sn) using SCAPS Software
ON-090	**Chikh Ali.Hadji**	ab initio study of the structural and electronic and Optical properties of The New Double Perovskite

ON-091	**Abdallah Timmaoui**	Electrochemical characterization of the AMX anion exchange membrane in buffered solution.
ON-092	**Bourega Mohammed**	The influence of nanoparticles on the behavior of droplet generation.

Partners

Speakers Abstracts

AOURAG HAFID

PROFESOR

CONTACT

h_aourag@mail.univ-tlemcen.dz

SMRIS-CRTI, Oran, Algérie

SHORT BIOGRAPHY

- *Professor Aourag Hafid: An Eminent Algerian Scientist*
- *Professor Aourag Hafid is a leading figure in the Algerian scientific community. Holder of a State Doctorate in physical sciences obtained at the University of Oran, he then led an exceptional academic and administrative career.*
- *Until 2001: Teacher-researcher at the University of Sidi Bel Abbès*
- *Period: 2000 – 2001: Rector of the University of Sidi Bel Abbès After holding the prestigious position of Rector at the University of Sidi Bel Abbès from 2000 to 2001, Professor Hafid joined the University of Technology of Belfort-Montbéliard in France as Professor*
- *from 2001 to 2003. He then continued his teaching and research activities, specializing in the field of quantum physics, at the Abou Bekr Belkaid University of Tlemcen from 2003.*
- *From 2008 to 2022, Professor Hafid served as Director General of the General Directorate of Scientific Research and Technological Development (DGRSDT) in Algeria. In this key role, he was instrumental in the development and promotion of scientific research in the country.*
- *Currently, Professor Aourag Hafid holds a position as Professor at the Industrial Technologies Research Center (CRTI) in Oran, where he continues his teaching and research activities in quantum physics.*
- *In recognition of his exceptional services in the field of scientific research in Algeria, Professor Hafid was honored with numerous tribute ceremonies organized by the country's various academic institutions and research centers.*
- *Throughout his remarkable career, Professor Aourag Hafid has been lauded for his exceptional scientific achievements and received numerous national and international honors, making him one of the most prominent Algerian scientists of his generation.*

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Pourquoi l'innovation en Science des Matériaux est très difficile ?

H. Aourag

Abstract

Even though today it is possible, thanks to artificial intelligence, big data and quantum mechanics, to discover thousands of new materials in one click.

However, any discovery becomes an innovation only if it has market value and this transition from laboratory to market can take more than 20 years. It is generally accepted that one of the main problems in commercializing new materials is the difficulty of moving from R&D to commercial production.

A multitude of obstacles must be overcome to achieve successful commercialization of a material. In general, these barriers can be classified as technical, such as the availability of testing procedures and property data, processing and manufacturing technologies, and susceptibility to material and process defects; regulatory/legal, such as public procurement policies, intellectual property rights, environmental protection, health and safety; and economic, such as R&D costs, market size, interest rates, investment costs and profit targets.

This conference will review all of these obstacles and the means of supervising all stages and will show that the term innovation is not so simple in materials sciences.

JELLALI SALAH

PROFESOR

CONTACT

s.jelali@squ.edu.om

Sultan Qaboos University, Oman

SHORT BIOGRAPHY

Dr. Eng. Salah Jellali currently holds the position of senior researcher in Water & Environmental Engineering at the Centre for Environmental Studies and Research (CESAR) at Sultan Qaboos University, Oman. His primary research focus revolves around local management and governance of solid and liquid wastes within the framework of circular economy and sustainability. A key area of his expertise involves the conversion of organic biomasses into high-value products such as biofuels, digestate, and biochars through pyrolysis or anaerobic digestion processes. Dr. Jellali has coordinated and participated in various national and international projects centered on the reuse of biochars as efficient adsorbents for wastewater treatment and/or as biofertilizers in agriculture. Additionally, he has actively contributed as a member of organizing and scientific committees for numerous international conferences on water and environment. Dr. Jellali has supervised several PhD theses and Master's students and co authored over 120 peer-reviewed scientific papers book chapters and books. Most of them are dealing with sustainable management of solid and liquid wastes within the context of circular economy.

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Biomass and mineral wastes turning into valuable biochars: Application for phosphorus recovery from actual wastewater

Salah Jellali[1,*],
Malik Al-Wardy[1], Jamal Al-Sabahi[2],Helmi Hamdi[3], Zohra Bengharez[4], Maram Al-Balushi[1], Majida Al-Harassi[1], Ahmed Al-Raeesi[1], and Mejdi Jeguirim[5]

1: Centre for Environmental Studies and Research (CESAR), Sultan Qaboos University (SQU), Oman;
2: College of Agricultural and Marine Sciences, SQU, Oman.
3: Center for Sustainable Development, College of Arts and Sciences, Qatar University, P.O. Box 2713, Doha, Qatar
4: Laboratory of Advanced Materials and Physicochemistry for Environment and Health, DjillaliLiabes University, Sidi Bel Abbes, Algeria
5: The institute of Materials Science of Mulhouse (IS2M), University of Haute Alsace, University of Strasbourg, CNRS, UMR 7361, Mulhouse, France
*: corresponding author. s.jelali@squ.edu.om

Abstract

Huge amounts of organic or mineral solid wastes are annually produced worldwide. Even their richness in resources, an important fraction of these wastes is still incinerated and/or landfilled.Moreover, phosphates (P) reserves which are vital for humans, animals and crops growthwould be seriously depleted before the end of the current century(Cordell et al., 2009). At the same time, large amounts of P are annually discharged in wastewaters with an important risk of surface water bodies quality deterioration(van Puijenbroek et al., 2019). Therefore, P and other nutrients recovery from wastewaters by using mixed solid wastes-derived biochars is considered as an innovative and promising approach that significantly contribute to the achievement of international initiatives regarding sustainability and circular economy concepts promotion(Jellali et al., 2022; Parasana et al., 2022).

In the current work, calcium- and magnesium-rich biochars were derived from the co-pyrolysis of abundant lignocellulosic (date palm fronds) and animal biomass (poultry/cow manure) and mineral wastes powder (marble/dolomite) at different ratios (from 0% to 50%) and pyrolysis temperatures (from 500 to 900 °C). These biochars were deeply characterized and then applied for P recovery from synthetic solutions and actual wastewater under batch, laboratory column and continuous stirring reactors (CSTRs).The effect of P initial concentration, biochar mass (or bed height), and flow rate (contact time) on P recovery

efficiency was precisely assessed. Moreover, the involved mechanisms were explored through various analyses of the biochars before and after P recovery.

Biochars characterization results indicate that the corresponding physico-chemical properties depend on the feedstocks ratios and also on the pyrolysis temperature. For instance, the best biochars properties were obtained for the highest temperature (900 °C). At this temperature, the surface area, pH of zero-point charge, and calcium content were assessed to be 52.3 m^2/g, 13.5, and 324 mg/g. The application of the synthesized biochars for P recovery show that this process is significantly enhanced with the increase of the pyrolysis temperature and also the marble or dolomite percentage. Moreover, the highest recovery efficiency was measured in batch mode for marble-modified biochar (about 145 mg g-1)(Jellali et al., 2024b). Due to the reduction of contact time between the P anions and biochar particles, this efficiency was reduced in column mode to around 80 mg/g. Moreover, P recovery process in column mode is jointly affected by biochar bed height, the initial P concentration and the flow rate. In CSTR mode, the P recovery performance by the marble-modified biochar depends mainly on the biochar mass and the initial P concentration. In this mode, and for both synthetic solution and wastewater effluent, an excellent P recovery was observed. Indeed, the P recovered amount in this mode was 43% higher than that observed in column assays. Moreover, owing to its richness in Ca cations, the P recovery from treated urban wastewater (109 mg/g) was 14% higherthan that observed for synthetic solution. It is also much higher than various raw and modified biochars (Jellali et al., 2024a).

Based on specific analyses (Fourier transform infra-red, X-ray diffraction, andpH of zero-point charge), the P recovery process was found to include combination of several mechanisms including electrostatic interactions, complexation and mainly precipitation as hydroxyapatite ($Ca_5(PO_4)_3OH$).

We can conclude that Ca-rich biochar can be considered as promising material for P recovery from actual wastewater. In real cases, this operation may be ensured P through the implementation of a CSTR followed by a decantation device after the secondary treatment step in existing wastewater treatment plants. The P-loaded biochar, collected at this decantation device, could be valorized in agriculture as slow release fertilizer instead of the commercial synthetic ones.

References

Cordell, D., Drangert, J.O., White, S., 2009. The story of phosphorus: Global food security and food for thought. Glob. Environ. Chang. 19, 292–305. https://doi.org/10.1016/j.gloenvcha.2008.10.009

Jellali, S., El-Bassi, L., Charabi, Y., Uaman, M., Khiari, B., Al-Wardy, M., Jeguirim, M., 2022. Recent advancements on biochars enrichment with ammonium and nitrates from wastewaters: A critical review on benefits for environment and agriculture. J. Environ. Manage. 305, 114368. https://doi.org/10.1016/j.jenvman.2021.114368

Jellali, S., Khiari, B., Al-balushi, M., Al-harrasi, M., Al-sabahi, J., 2024a. Novel calcium-rich biochar synthesis and application for phosphorus and amoxicillin removal from synthetic and urban wastewater : Batch , columns , and continuous stirring tank reactors investigations. J. Water Process Eng. 58, 104818. https://doi.org/10.1016/j.jwpe.2024.104818

Jellali, S., Khiari, B., Al-balushi, M., Al-sabahi, J., Hamdi, H., Bengharez, Z., Al-abri, M., Al-nadabi, H., Jeguirim, M., 2024b. Use of waste marble powder for the synthesis of novel calcium-rich biochar : Characterization and application for phosphorus recovery in continuous stirring tank reactors. J. Environ. Manage. 351, 119926. https://doi.org/10.1016/j.jenvman.2023.119926

Parasana, N., Shah, M., Unnarkat, A., 2022. Recent advances in developing innovative sorbents for phosphorus removal—perspective and opportunities, Environmental Science and Pollution Research. Springer Berlin Heidelberg. https://doi.org/10.1007/s11356-022-19662-5

van Puijenbroek, P.J.T.M., Beusen, A.H.W., Bouwman, A.F., 2019. Global nitrogen and phosphorus in urban waste water based on the Shared Socio-economic pathways. J. Environ. Manage. 231, 446–456. https://doi.org/10.1016/j.jenvman.2018.10.048

YARUB AL-DOURI

PROFESOR

CONTACT

yaldouri@yahoo.com

Technology Innovation Institute, Abu Dhabi, United Arab Emirates

SHORT BIOGRAPHY

Prof. Dr. Yarub Al-Douri is a Fellow of European Academy of Sciences. Al-Douri is winner of the prestigious Khalifa International Award for Date Palm and Agricultural Innovation 2024. He has initiated Nanotechnology Engineering MSc Program and Nano Computing Laboratory. He has received numerous accolades including winner of IAAM Scientist Award by International Association of Advanced Materials, Sweden 2022, World's Top 2% Scientists by Stanford University, USA 2023, 2022, 2021 & 2020, World's Top 2% Scientist Career-Long Citation Impact by Stanford University, USA 2020, OeAD Award, Austria 2020, Japan Society for the Promotion of Science (JSPS) Award 2019, Asian Universities Alliance (AUA) Award 2019, the total is 75 awards. Al-Douri is Associate Editor of Nano-Micro Letters (Q1,IF=26.6,Springer), Editor-in-Chief of Experimental and Theoretical NANOTECHNOLOGY, Editor-in-Chief of World Journal of Nano Science and Engineering. His research field focuses on nanotechnology, renewable energy, nanoelectronics, nanomaterials, modelling and simulation, semiconductors, optical studies. Finally, Al-Douri is a public figure at international media in the UK, Singapore, Malaysia, Qatar and UAE. Al-Douri has more than 860 publications including Citations < 12000, h-index = 60, i10-index = 243 and US$ 5.1M research grants. Finally, Al-Douri is one of the Middle-East, North of Africa, Malaysia and Southeast Asia's most renowned scientists known for his contributions in Nanotechnology and renewable energy, and a public figure at international media in the UK, Singapore, Malaysia, Qatar and UAE.

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Future prespective of nanotechnology : Industial and biomedical application

YARUB AL-DOURI

Abstract

The nanotechnology could deliver world-altering changes in the ways we create, transmit, store, and use energy. The scientists are working to develop super-efficient batteries, low-resistance transmission lines, and cheaper solar cells. However, the likelihood and time frame of these developments is unknown for the moment. The next generation of solar cells is thin film solar cells—flexible sheets of solar panels—that are easier to produce and install, use less material, and are cheaper to manufacture. These sheets can be incorporated into a briefcase that charges your laptop, woven into wearable fabrics that charge your cell phone and iPod, or incorporated into windows that can supply power to high-rise buildings. In different parts of the world, the people do not have access to safe drinking water. But the new nanofiber water filters can remove bacteria, viruses, heavy metals and organic materials from water. They are re relatively inexpensive and easy to use, so the nanofilter could be widely employed easily. Providing pure drinking water would help prevent disease in many parts of the world, but it would not resolve many basic inequalities. The nanotechnology has unique properties. The electrical properties, durability, strength and activity of nanomaterials are enhanced and engineered to obtain desired features through nanotechnology. Nanotechnology focusses on solar, hydrogen and biomass energy. The nanostructured catalysts are used to increase the efficiency of fuel cells while porous nanomaterials are used for hydrogen storage. The quantum dots and carbon nanotubes increase the energy absorption properties of solar cells. The development of cost-effective renewable energy systems will contribute to the urgent energy goals of our world and reduce the destructive effect of human activities.

AMAR TILMATIN

PROFESOR

CONTACT

atilmatine@gmail.com

Univ. Of Sidi Bel-Abbés

SHORT BIOGRAPHY

- *Amar Tilmatine is an electrical engineer, graduated from the University of Sciences and Technologies of Oran in 1988 as a state engineer, and in 1991 with a Magister specialized in high voltage. He then continued his studies and obtained his doctorate in 2004 at the Department of Electrotechnics of the Djillali Liabes University of Sidi-Bel-Abbès, specializing in applied electrostatics. In 2010, he was promoted to the rank of professor . He is also a "Senior member" of the IEEE association and was former president and co-founder of the IEEE Algeria section and the Algerian association of electrical and electronic engineering AAGEE. He is also a founding member of the Algerian Academy of Sciences and Technology AAST.*
- *He is currently director of the APELEC laboratory, and is also responsible for the "Industrial Technologies" technological platform of the University of Sidi-Bel-Abbès, continuing his commitment to the practical application of scientific research in the industrial world. has filed 21 invention patents, including one in 2022 in PCT with international extension, relating to a new technique for cleaning solar panels. His scientific areas of interest cover high voltage, electrostatics and plasma applications. Amar has published more than 190 scientific papers and is the author of two books titled "Electromagnetic Field Theory" and "High Voltage Techniques".*
- *In collaboration with its laboratory partners, Amar Tilmatine has obtained promising results in the socio-economic sector, notably with research projects on electrostatic smoke filters, electrostatic separators, water treatment with ozone and ozone disinfection.*

Séparateurs électrostatiques des particules: application à la récupération des matériaux plastiques et métalliques

Amar Tilmatine

Abstract:

The conference will focus on the operation and applications of electrostatic particle separators in the recycling of materials from waste electronic and electrical equipment. These devices use physical properties, including electrical conductivity and particle density, to facilitate their separation. Under the effect of an intense electric field, electrically charged materials are attracted to electrodes of opposite polarities, allowing effective separation between conductive and insulating components. The presentation will cover three main types of separators: those suitable for mixtures of "metal/plastic" particles, those intended for mixtures of different types of plastics (such as PVC and PE), as well as separators dedicated to sorting metal particles such as as copper and aluminum.

BÉCHIR HAMROUNI

PROFESOR

CONTACT

+216 98 686 710

bechir.hamrouni@fst.utm.tn

Faculty of Sciences
of Tunis, 2092
Manar 1, Tunis,
TUNISIA

SHORT BIOGRAPHY

Emeritus Professor at the University of Tunis El Manar, since May 2023. He is Founder and head of Research Laboratory "Desalination and Water Treatment", 2011-2022. He is Founding President of the Tunisian Desalination Association He is a state doctorate (Doctorat d'État) in Analytical Chemistry from the University of Tunis El Manar and has a PhD Thesis and a master (DEA) in Analytical Chemistry from Pierre and Marie-Curie University (Paris VI). He is organizer and chairman of 10 scientific conferences, author and co-author of 114 papers including 94 in impact factor journals, author and co-author of 9 books and 2 book chapters with ISBN codes. He participated in several national and international research projects and is a frequent invited speaker on water and filtration related topics. He supervised 28 Doctoral Thesis (25 defended, 03 in progress) and 41 Research Masters supported. He has been coordinator of two Research Masters: Master's "Analytical chemistry", Faculty of Sciences of Tunis, 2009-2018 and Master's "Integrated Water Management", Faculty of Sciences of Tunis, as part of the Erasmus+ MAYA project, 2018-2021.

Chemistry and materials science to cope with water scarcity

Béchir Hamrouni

Abstract:

North Africa countries suffer from severe water scarcity where wateravailabilityismuch lower than 1000 m^3/year/habitant. This situation will get worse because of climate change (increase of temperature, decease of rainfall). Hence the obligation to use unconventional resources, especially Water Desalination. This requires a strategy relating to awareness, to training and research.In this context, chemistry, materials science and engineering play a critical role in developing innovative solutions to address water scarcity and ensure access to clean and safe water for all. By continuously researching and developing new materials and technologies, scientists can help mitigate the impacts of water scarcity and contribute to sustainable water management practices.

The state of the art of water desalination as a solution to water supply is reviewed. All stepsof a desalination plant, namely salt water intake, pre-treatment, desalination processes and its energy consumption, brine rejection and the post-treatment are the subject of various research projects. At this level, our role as academics is important to contribute and conduct research activities on pollutants removal, membrane materials, corrosion resistance, energy efficiency, sustainability, cost reduction, environment impact, …

SAMIR ROMDHANE

PROFESOR

CONTACT

samir.romdhane@fst.utm.tn

Tunis El Manar University, Tunisia

SHORT BIOGRAPHY

Laboratory of Advanced Physics and Quantum Phenomena Faculty of Sciences of Tunis, Tunis,Tunisia. Born: April 24, 1966 Samir Romdhane studied physics at the Faculty of Sciences of Tunis, where he was graduated in 1989. He received a doctor's degree from the Faculty of Sciences of Tunis in 1997. He obtained the Habilitation in physics in 2003. Scientific interests deal with the electronic properties of organic conjugated materials and their applications in organic electronics, in particular in the field of solar energy conversion into electric energy. The research activity is mainly focused on the investigation of organic solar cells, with the aim to understand the complex interplay between the chemical structure of materials, their chemical-physical properties and their effects on the performance of solar cells

Organic Solar Cells : Material Innovations for a Sustainable Energy Future

Samir Romdhane

Abstract

The quest for sustainable and renewable energy sources has intensified in response to the escalating global energy demands and the urgent need to mitigate climate change. Organic solar cells (OSCs) have emerged as a promising alternative to traditional silicon-based photovoltaics due to their potential for low-cost production, lightweight and flexible applications, and tunable properties. This talk will delve into the recent material innovations driving the advancements in OSC technology, with a special focus on the breakthroughs achieving over 19% ¬[1-2] power conversion efficiency (PCE).

Key focus areas will include the development of novel organic semiconductors, the optimization of donor-acceptor materials, and the enhancement of device architectures. Breakthroughs in non-fullerene acceptors, conjugated polymers will be highlighted, showcasing how these materials contribute to the significant increase in PCE and operational stability. We will provide insights into the underlying mechanisms and material properties that enabled these improvements.

The talk will also address the critical role of structural organization in enhancing OSC performance [3]. Innovations in the morphological control of active layers will be discussed. These structural optimizations have been pivotal in improving charge transport, reducing recombination losses, and maximizing light absorption, thereby significantly boosting overall device efficiency.

By examining these cutting-edge innovations and their practical applications, we aim to provide a comprehensive overview of the current state and future prospects of organic solar cells, underscoring their significance in achieving a sustainable energy future.

Reference

[1] Jiehao Fu et al… Nat. Com. (2023) 14:1760

[2] Baobing Fan et al… Joule 8, 1443–1456, May 15, 2024

[3] Congqi Li et al… J. Am. Chem. Soc. 2022, 144, 14731−14739

MATTHEUS GOOSEN

PROFESOR

CONTACT

mgoosen@alfaisal.edu

Alfaisal university,
Saudi Arabia

SHORT BIOGRAPHY

Professor Mattheus (Theo) Goosen currently serves as the Associate Vice President for Research & Graduate Studies at Alfaisal University in Riyadh Saudi Arabia, a position he has held for the past 16 years. He was also the Acting Dean of the College of Science & General Studies from 2017 to 2022. In 2024 he was appointed as the Secretary General of the University Council. As one of the founding senior faculty he feels extremely proud to be part of this competent, diverse, and internationally renowned institution. Alfaisal University is a fully accredited NCAAA institute of higher education. Furthermore, the Times Higher Education (THE) Young Universities 2022 Rankings placed Alfaisal University 1st in Saudi Arabia, 1st in the Arab Region & 36th ,Globally. The university was also ranked 8th by THE in "The World's Best Small Universities" (2022).

Prior to joining Alfaisal University, Dr Mattheus acquired extensive academic experience working for several prestigious Institutions over a span of more than 40 years. He was the Campus Dean of the New York Institute of Technology (NYIT) in Amman, Jordan (2006-2008). Before this he worked in Puerto Rico, USA as the Dean of the School of Science and Technology at the Universidad del Turabo (2004-2006). Other Institutes where he has held academic positions were Sultan Qaboos University, Muscat (1994-2004), Oxford University, UK (sabbatical 1990- 91), Queen's University, Kingston, Canada (1984-1996). Apart from pedagogical job roles, Dr Mattheus has also held various technical positions in respected companies such as Areej Vegetable Oils & Derivatives (Oman), Oman Agricultural Development Company (Oman) & Connaught Laboratories Limited (Canada ON).

Dr. Mattheus has been awarded several accolades and scholarships for his achievements. He was recognized for example in the "Stanford University's World's Top 2% Scientists List" (Career Impact) in 2023. He still teaches a course on "Environmental Science & Sustainability" to undergraduate students. Additionally, Dr Mattheus has more than 200 publications to his credit including over 150 refereed journal papers, 45 conference papers, 12 edited books and 10 patents. He has been involved in major research projects and has helped to raise over $20 million USD for research work. His areas of research interests include renewable energy, desalination, sustainable development, membrane separations, biomaterials, and culinary innovation & development.

Sustainable Development, Renewable Energy& Advanced Materials Research

MATTHEUS GOOSEN

Abstract:

Sustainable growth using renewable energy sources is now considered by both the private and public sectors as being the model to follow. The use of advanced materials research is essential to meet the growing demand for applications such as water desalination. Furthermore, the expansion of renewable energy sources to run commercial processes at a larger scale is hampered by technical, economic, regulatory and environmental challenges including new material development. This critical review focusses on integrated approaches in using renewable energy such as solar technologies for water desalination. Innovative and sustainable processes which are suitable for integrated renewable energy systems are also presented, along with the benefits of these technologies and their limitations. The market potential, environmental concerns, regulatory & socio-economic factors are likewise evaluated as well as the need for accelerated development of renewable energy-driven technologies. The role of advanced materials in providing a possible solution to the global plastic pollution problem is also discussed.

Oral Communications

O-01

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Predictive properties of the nickel sulphide NiS

Abderrahmane Reggad[a]

[a] Science and Technology Department, Technology Faculty, University of Chlef

Abstract:

We have made a predictive study using the rules of crystal chemistry to determine the possible crystal structures to be adopted by the nickel sulfide NiS. To check these possible structures MnP, NaCl and ZB we have done an ab initio calculation using the wien2k code within the DFT approach and the hybrid functional. We have also studied the magnetic natures of these structures as the possible existence of the half metallicity in the ferromagnetic state in ZB structure.

Key words: ***Prediction****; NiS; half metallicty; antiferromagnetic; crystal chemistry.*

Corresponding Email: abde.reggad@gmail.com

References

[1] A. Reggad, R. Lardjani, R. Baghdad, B. Bouhafs, Physica B 526 (2017) 89e95.
[2] Tsubokawa. J. Phys. Soc. Jpn 13 (1958) 1432.
[3] P. Blaha, K. Schwarz, G. Madsen, D. Kvasnicka, J. Luitz, WIEN2k, An Augmented Plane Wave + Local Orbitals Program for Calculating Crystal Properties (Karlheinz Schwarz, Techn, Universität Wien, Austria, 2001.

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Experimental Evaluation of Boron Carbide-Based Nanocomposite for Nuclear Shielding Against Highly Ionizing Radiations

Abdous Slimane[a]*, Derradji Mehdi[a], Khiari Karim[a], Mehalli Oussama[a], Habes Abdelmalek[a]

[a] UER Procédés Energétiques, Ecole Militaire Polytechnique, BP 17, Bordj El-Bahri, Algiers, Algeria

Abstract:

Nuclear energy is regarded as one of the most low-carbon energy sources, emitting secondary radiation that can harm human safety and materials [1-3]. The path towards attenuating these highly ionizing radiations is centered on developing lightweight, low-cost shields based on polymeric precursors [4, 5]. However, the design of lightweight neutron shields has been restricted for quite some time to using epoxy thermosets as the main building blocks. Meanwhile, the recent developments in the field of polymers suggest otherwise. Benzoxazine (Bz) resins have taken the lead over traditional thermosets in many exigent applications. Therefore, in a vision to introduce newer matrices with better performances and to further expand the applications of the Bz resins into the nuclear field, the neutron shielding efficiency and the thermal resistance performances of the neat Bz polymer and its subsequent silane surface-modified nanometric B_4C-reinforced composites were investigated. The neat Bz polymer displayed better thermal neutron screening performances than the epoxy with a macroscopic cross-section (Σ) of 3.3878 cm^{-1}. The effects of the particle amount and size were also studied to maximize the shielding ability of the developed materials. For instance, the Bz composite containing 5 % wt of B_4C displayed an outstanding screening ratio of about 97.78 % for a sample thickness of 11 mm. Finally, the remarkable findings were put into context by providing multifaceted comparisons with the conventional shielding materials.

Key words: Nano-composites, Nuclear Energy, Radiation shielding, Boron Carbide

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Title: **Terpolymer of Propylene Oxide - Styrene- Methyle Methacrylate**

Mohamed BENADDA[a], Karima OUSSADI[b,]

[a] Université d'Oran 1 Ahmed Benbella, Faculté des Sciences exactes appliquées, Département de Chimie, Laboratoire de Chimie des Polymères, BP 1524 El M'Naouar, 31000 Oran, Algerie

[b] Université des Sciences et de Technologie Mohamed Boudiaf, Faculté de Chimie, Département de Génie des Matériaux, Laboratoire de Physico-Chimie des Matériaux Catalyse et Environnement (LPMCCE), BP 1505 El M'Naouar, Oran, Algérie

Abstract:

Text of the abstract A green synthetic route is proposed to obtain polyterpolymerisation with a controlled structure, by using maghnite-H^+. It is an environmentally friendly heterogeneous catalyst. The maghnite-H^+ is an Algerian clay, characterized by very high specific surface. The synthesis of a new terpolymer of propylene oxide (PO) with styrene (St) and Methyle Methacrylate (MMA) by cationic polymerization is reported. The terpolymerization was performed in bulk at temperature 20°C. The terpolymer was prepared by the reaction of propylene oxide with styrene and Methyl Methacrylate in the presence of natural Algerian montmorillonite clay modified by 0.05-1 M of H_2SO_4, known as Maghnite-$H^{+1,2}$. It is a proton source, a non-toxic and an efficient catalyst for cationic polymerization of many vinylic and hetero-cyclic monomers. The structure of the products obtained is confirmed by 1H-NMR, Fourier transform infrared spectroscopy, gel-permeation chromatography. The yield of terpolymerization depends on the amount of Mag-H^+ used and the reaction time.

Key words: Catalyst, Clay, Environment, Terpolymerisation.

Corresponding Email: e-mail: benadda_mohammed@yahoo.fr

References

[1] M. Benadda, M. I. Ferrahi, M. Belbachir, Bull. Chem. Reac. Eng. & Catal, 9 (3), 201-206, **2014.**
[2] K. Oussadi ; V. Montembault ; M. Belbachir ; L. Fontaine, Journal of Applied Polymer Science, Vol. 122, 891–897, **2011**

.

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Bending behavior of sandwich structures with glass and carbon fiber skins and PVC foam cores

REZIG Naima[a], HALIMI Amel[b], MANSOURI Essaid[a,b], KESSOUAR Mohamed Yazid[a]

[a] Ecole Supérieure des Techniques de l'Aéronautique, Dar El Beida, Algérie.
[b] Laboratoire Génie des Matériaux, Ecole Militaire Polytechnique, Bordj El Bahri, Algérie.

Abstract:

The present paper describes an experimental investigation aimed at measuring the bending mechanical properties of a sandwich material. The latter is composed of a PVC foam core called 'Airex C50.70' with thin glass laminate and carbon laminate skins, respectively. The studied materials were realized at the laboratory using the vacuum technique and epoxide resin. Then, the obtain plaques were divided into standardized samples based on the planned experiment. Subsequently, the sandwich panels, which may be categorized as either glass or carbon, underwent testing using both three- and four-point bending methods. Subsequently, an analysis was conducted to compare the outcomes achieved based on the bottom and higher arrangement of the PVC core.

Keywords: Sandwich, PVC foam, laminate, glass, carbon, bending.

Introduction:

The exponential increase in the utilization of composite materials in recent years has generated significant hope. Composite constructions have become prominent in various industrial sectors, including aeronautics, aerospace, land and marine transport, and recreational products and equipment. The incorporation of sandwich materials has yielded significant benefits in terms of enhanced strength, reduced weight, and improved thermal and acoustic insulation. Nevertheless, the selection of materials composing the layers and the adherence between them is crucial to ensure the necessary mechanical functionality. Comprehensive investigations are thus required to evaluate their behavior under specified loading conditions. In this context, the present work is focused on analysing the mechanical characteristics of two sandwich structures consisting of a PVC core and two skins made of glass/epoxy and carbon/epoxy laminates respectively. Hence, a thorough examination and analysis of the flexural properties of the research materials in both three-point and four-point bending configurations is conducted and subsequently deliberated upon.

Experimental procedure

In this work, we fabricated two Airex 50.70 PVC foam sandwich sheets by employing the vacuum process and utilizing epoxy resin as an adhesive to bond the core and the skins. We have selected two types of composites for the skins: a laminate consisting of three layers of glass twill and another one made of carbon taffeta. Subsequently, we sliced our samples in accordance with the guidelines outlined in standard NFT54-606. Subsequently, Zwick Z005 universal machine was used to conduct three- and four-point bending tests (Figure 1).

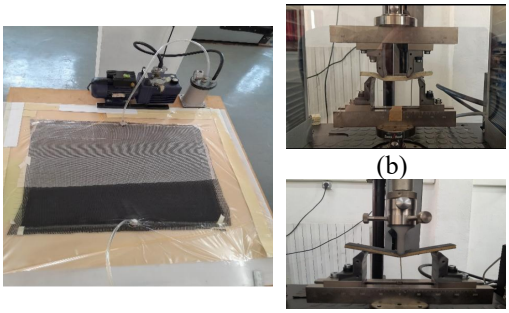


Figure 1: (a) Manufacture of sandwich panels from PVC foam, and Bending systems: (b) Three and (c) four points.

Results and discussion

The elaborated sandwich panels were subjected to testing in line with the NF T 54-606 standard as part of this experimental investigation. Three specimens were evaluated for each test to verify the reproducibility of the acquired results. In order to analyze the impact of the glass fiber reinforcement on the upper surface of the PVC foam, we positioned the test specimens in two locations: upper and lower. Figures 3 and 4 illustrate the contrasting outcomes of the three point bending tests on the two sides of the two sandwich materials. Regarding the carbon sandwich, it is evident that the produced curves exhibit brittle behavior in the three point bending test conducted on both the upper and lower aspects. Nevertheless, the maximum stress exerted on the lower facet is nearly identical to the load exerted on the bottom facet. This finding unequivocally demonstrates that the orientation of the load does not have a significant impact on the behavior of the carbon sandwich.

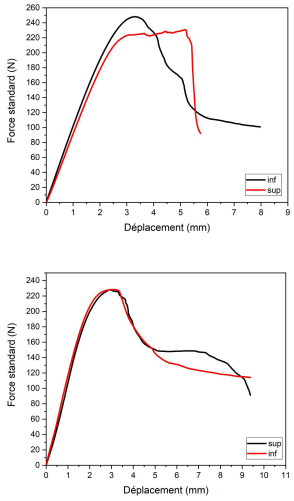


Figure 3: Bending curves along the upper and lower facets for the (a) glass and (b) carbon skin.

Conclusion:

This study presents the findings from conducting three-point and four-point bending tests on two sandwich materials composed of glass and carbon fiber skin, respectively. The test findings demonstrated the impact of the material aspect exclusively on the glass sandwich. The overall flexural strength of the carbon sandwich was not affected by the direction of loading. The determined shear modulus values of the core for both types of sandwich exhibit a high degree of similarity, suggesting that the conducted tests are in strong concurrence. This result also confirms the figure provided in the technical data sheet for the PVC core.

Corresponding Email:
Rezignaima.ait@gmail.com

References

[1] Mahrsi, K. (2021). Etude expérimentale et numérique du comportement mécanique de la mousse PVC sous chargement monotone et cyclique (Doctoral dissertation, Nantes).

[2] Far, H., & Nejadi, S. (2021). Experimental investigation on flexural behaviour of composite PVC encased macro-synthetic fibre reinforced concrete walls. Construction and Building Materials, 273, 121756.

[3] Garay, A. C., Souza, J. A., & Amico, S. C. (2016). Evaluation of mechanical properties of sandwich structures with polyethylene terephthalate and polyvinyl chloride core. Journal of Sandwich Structures & Materials, 18(2), 229-241.

[4] Uzay, C., Geren, N., Boztepe, M. & Bayramoglu, M. (2019). Bending behavior of sandwich structures with different fiber facing types and extremely low-density foam cores. Materials Testing, 61(3), 220-230.

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Study on the elimination of various pollutants using carbon-based materials

Mohammed Elamine MERABTI[a,c,d], Omar KHELIFI[a,b,c]

[a] Department of Hydrocarbons and Renewable Energy, Faculty of Science and Technology, Ahmed Draïa Adrar University, 01000 Adrar, Algeria
[b] Laboratory of Industrial Analysis and Materials Engineering (LAIGM), Department of Process Engineering, Faculty of Science and Technology, University 8 May 1945 Guelma, BP 401, Guelma 24000, Algeria
[c] Catalytic Materials and Industrial Processes Laboratory (LMCPI), Faculty of Science and Technology, Ahmed Draïa Adrar University, 01000 Adrar, Algeria
[d] Energy, Environment and Information Systems Laboratory (LEESI), Faculty of Science and Technology, Ahmed Draïa Adrar University, Algeria

Abstract:

The aim of this study is to assess the potential of activated carbon derived from Washingtonia fruit pits for adsorbing paracetamol and sodium diclofenac in aqueous solutions. The physicochemical properties, as well as the morphological and structural characteristics (BET, SEM, and FTIR) of the prepared activated carbon, were determined. Adsorption experiments were conducted by adjusting various operational parameters (initial concentration, contact time, and temperature). Isothermal and kinetic models were applied to analyze the experimental data, showing that the Freundlich model and pseudo-second-order model are most suitable. Optimal conditions were determined to achieve maximum adsorption capacities of 21.0742 $mg.g^{-1}$ for paracetamol and 48.268 $mg.g^{-1}$ for sodium diclofenac. The results suggest that activated carbon prepared from Washingtonia fruit pits can be beneficially used for the adsorption of pharmaceutical products from aqueous solutions.

Keywords: Adsorption, activated carbon, Washingtonia fruit pits, paracetamol, diclofenac.

Corresponding Email:
mmerabti@univ-adrar.edu.dz

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Cross-linked alginate biocomposite beads for Methylene Blue removal. Optimization study using a statistical approach based on a full factorial Design

Kheir Eddine KHODJA, Zohra BENGHAREZ

Laboratory of Advanced Materials and Physicochemistry for Environment and Health, Djillali Liabes University, Sidi Bel Abbes, Algeria

Abstract:

This study aimed to optimize the adsorption process for Methylene Blue (MB) using eco-friendly composite beads based on Algerian Arabic gum and sodium alginate. The investigation used a full factorial design to analyze the key factors that influence the adsorption process. Individual and interaction effects of pH, initial MB concentration, contact time, and bio-composite mass on MB removal efficiency were examined.

Analysis of variance (ANOVA) highlighted the significant impact of these factors with a P value < 0.05. In particular, contact time was found to be the most significant factor for MB removal, with a particularly low P value of < 0.0001.

A prescribed first-order regression model demonstrated a robust fit to the experimental data, resulting in a high coefficient of determination ($R^2 = 0.970$). The optimal conditions identified for maximum Methylene Blue removal are in close agreement with the predicted values from the statistical design.

This research provides valuable insights into the efficient removal of cationic dye using composite materials developed from natural resources. The study emphasizes their potential in water treatment and environmental remediation applications.

Key words: Alginate, composite beads, Methylene Blue, removal efficiency, experimental design, optimization.

Corresponding Email: khodjakheireddine@yahoo.com

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Title: Impact of the Pulsed Electric Field on the extraction of the phenolic compounds of an industrial plant: Eucalyptus globulus

Manel Nardjes Toumi[a], Abdelfettah Benyamina[a], Mohamed Ali Bouzidi[a], Abdelkader Semmak[b], Yassine Bellebna[b], Fawzia Toumi[a] and Amar Tilmatine[b]

[a]APELEC Laboratory, Djillali Liabes University of Sidi Bel-Abbes, Sidi Bel Abbes 22000, Algeria
[b] LEDE Laboratory, Djillali Liabes University of Sidi Bel-Abbes, Sidi Bel Abbes 22000, Algeria

Abstract:

Eucalyptus extract-based pharmaceutical products are widely used because of their medicinal properties and their rich content of secondary metabolites, mainly phenolic compounds. This study aimed to maximize the extraction yield of these compounds and reduce the extraction duration by using a pulsed electric field (PEF) level of 6 kV/cm. The pulse width (T), number of pulses (n), and solvent concentration [C] were analyzed. Several ethanolic extracts were obtained from the leaves of Eucalyptus globulus, and the content of total phenols, total flavonoids, and condensed tannins was measured through spectrophotometry. The results, obtained immediately after PEF treatment, revealed that for optimal values of the analyzed factors, the total phenol content doubled and the flavonoid content increased significantly. However, PEF pre-treatment had no effect on the tannin yield. Moreover, optimization was performed using the design of experiments methodology for identifying optimal values of the analyzed factors.

Keywords: Eucalyptus globulus, pulsed electric field, total phenol, flavonoids, condensed tannins.

Corresponding Email: manelnardjes_toumi@yahoo.fr

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Optimisation of the photovoltaic efficiency of a cell based on GaAs

Loubna Benhabib[a], Chafika Zidani[a]

[a]Department of physics, URMER laboratory, Aboubekr Belkaid university, Tlemcen, Algeria

Abstract:

Photovoltaic solar energy is a direct transformation of part of the solar radiation into electrical energy. This energy conversion is carried out by means of a solar cell whose efficiency depends on the range of the solar spectrum absorbed. Nowadays, thin-film solar cells are increasingly used mainly because of their low cost.

This work consists in simulating and modeling a solar cell based on the GaAs material. The simulation was carried out by the mathematical tool Matlab.

For this we have considered a GaAs-based cell already in theoretical and experimental study. The latter had a rate of return of 18.5% in theory and 19% in experimental [1]. Taking into account the ideal conditions of T=298K and solar intensity of 1000W/m², we have achieved a yield that is worth 19.2%, a value close to that obtained in experiments.

Outside, to deepen in the simulation, we considered a variation of some parameters that seemed to influence the characteristics of the cell such as: coefficient of absorption, density of electrons and factor of ideality. We have proceeded in such a way that each time we vary one parameter the other two are considered constant. For this, the influence of the factor of ideality with a value higher than that of the theory, led us to a higher yield of 25.5%. Therefore, by increasing the value of the coefficient of absorption, the value of yield fell by 20.1% compared to the influence of the factor of ideality but a value superior to the theory. Let us end by the influence of the density of electrons, or the decrease of the latter generates an increase in the efficiency that was worth 21.3% compared to the theory. The results obtained allowed us to model a cell based on GaAs with a yield of 29.8%. Then our simulation continued with a real study whose temperatures and solar intensities are those of January and December for the year 2021 in the Tlemcen region. Or yield to slightly decrease to become 24.3% [2]

Key words: photovoltaic, solar cell, GaAs, simulation, materials

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environnement

Methodology for converting GNSS measurements in to water vapour in the lower atmosphere.

Houaria Namaoui [a]

[a]Authors' Space of Geodesy, Center of Space Techniques, Algeria

Abstract:

Water vapour plays a fundamental role in the atmosphere, both in terms of climatology and meteorology. It is one of the main greenhouse gases because of its high radiative capacity and its interactions with clouds and aerosols. Its observation remains very partial because of its high spatio-temporal variability.

Numerous systems already exist, such as radiosondes, radiometers, lidars and airborne measurements, to study this variable. However, the data provided by these systems quickly reaches certain limits. Some instruments do not have sufficient spatial or temporal resolution to characterise the water vapour field. Others can only be used in good weather or under specific atmospheric conditions: radiosondes giving the vertical profile of water vapour are only taken twice a day, and the radiosonde sites are located several hundred km apart.

The electromagnetic signal transmitted by Global Navigation Satellite Systems (GNSS) undergoes a delay that is mainly caused by water vapour in the atmosphere. By estimating the zenith delay affecting signal propagation, it is possible to estimate the column of water vapour in the troposphere by knowing the temperature and pressure at each station.

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Modeling and Simulation of Heat Transfer by Natural Convection with Periodic Heat Source in Fluid-Structure Interaction System

Tarek NEHILA[1*], Elhadj BENACHOUR[1] Keltouma FELDJI[1], Khadidja ASNOUNE[1],Mohamed HASNAT[1]

[1]ENERGARID Laboratory, Tahri Mohamed University of Bechar, Tahri Mohamed University of Bechar, P.O. Box 417.08000, Algeria

Abstract:

In this investigation, natural convection heat transfer within a square cavity is addressed, involving the interaction between air (Pr = 0.71) and a thin, flexible, and oscillating conductive fin. The movement of the structure is captured using a moving mesh established through the Arbitrary Lagrangian-Eulerian (ALE) approach. The Finite Element Method (FEM) with the Galerkin's weighted residual approach is used to solve the equations.This study explores the effect of a cosinusoidal heat source on heat transfer. The dimensionless numerical results include the fin's location, as well as streamline patterns, isotherms, and the average Nusselt number. Fixed parameters include the Rayleigh number (Ra = 10^6), Young's modulus (E = 10^{11}), and a conductivity ratio of 10. The results indicate that an increase in the amplitude of wall undulation leads to an improvement in the heat transfer rate.

Key words: Numerical simulations; Fluid-Structure Interaction; Natural convection; Finite element modeling

Corresponding Email:

Nehila.tarek@univ-bechar.dz

O-11

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

THEORETICAL INVESTIGATION OF THE ANTI-ALZHEIMER POTENTIAL OF A NEW ORGANIC SUBSTANCE

Hasnia ABDELDJEBAR [a], Bilal BOUFEKANE [b], Yamina BELMILOUD [c], Meziene BRAHIMI [c]

[a] Centre de Recherche Scientifique et Technique en Analyses Physico-chimiques(CRAPC), BP 384, Bou-Ismail, RP 42004, Tipasa, ALGERIE.
[b] Université Belhadj Bouchaib Ain Temouchent, Faculté des Sciences et Technolgies, Département Agro-alimentaire, BP N101, Route de Sidi Bel Abbes, Ain Temouchent, 46000, ALGERIE.
[c] Laboratoire de Physico-Chimie Théorique et de Chimie Informatique. Université des Sciences et de la Technologie Houari Boumediene, Faculté de Chimie, BP 32 El Alia, Bab Ezzouar, Alger, 16111, ALGERIE.

Abstract:

Benzimidazolones are recognized as the preferred heterocyclic systems in medicinal chemistry. Their structures are characterized by a carbonyl group placed between two nitrogen atoms. This structural particularity gives them a considerable place in various fields, especially in pharmacology. They exhibit a wide range of biological activities and are used as building blocks for pharmaceuticals, agrochemicals, inhibitors, pigments, herbicides and fine chemicals [1]. In order to explore the biological activity of our new heterocyclic molecules derived from benzimidazolones, a computational study was performed using the autodockvina program as computer software [2]. The molecular docking of our ligands, whose spatial arrangement is slightly different due to the substitution of the base ring, shows that the studied protein-drug structures exhibit the same degree of inhibition towards Alzheimer's disease, reflected by very similar docking scores, as well as a good target-ligand affinity. These interesting results need to be studied in more detail to understand their potential in the treatment of this disease.

Key words: Benzimidazolone, Alzheimer, molecular docking, pharmaceutical potential.

Corresponding Email: abdeldjebar_hasnia@yahoo.com

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

ESSAI D'ADSORPTION DU CADMIUM PAR UN CHARBON ACTIF ISSU D'UN DECHET AGROALIMENTAIRE

Khadidja CHIALI CHARIF[a], Mohamed SIDHOUM[b], Nadia RAMDANI[c], Mokhtar BOUNAZEF[d]

[a] Département sciences de l'environnement, Laboratoire matériaux et catalyse, *UDL SBA ,ALGERIE*
[b] Institut des sciences agronomiques, Laboratoire de Génétique Appliquée en Agronomie, Écologie et Santé Publique, *UDL SBA ,ALGERIE*
[c] Département génie des procédés, laboratoire APELEC, *UDL SBA ,ALGERIE*
[d] Département génie mécanique, *UDL SBA ,ALGERIE*

Resume:

Dans cette étude nous nous sommes intéressés à un déchet classé parmi les déchets dangereux il s'agit des batteries (piles à cadmium) usées, qui beaucoup d'études révèlent la présence d'importante quantité de cadmium qui dépasse les normes.
Afin de réduire ce métal lourd, On propose l'adsorption en utilisant un charbon issue d l'agroalimentaire (son de blé).
Le son de blé à été utilisé pour préparer du charbon, différent charbon ont été préparés pour réaliser une adsorption (à titre comparatif) sur une solution contenant des ions cadmium (Cd^{2+}). Le charbon calciné à 650°C et activé chimiquement par l'acide phosphorique a donné les meilleurs résultats en termes d'adsorption (3,54 mg/g).
Malgré un taux d'adsorption inferieur a d'autre matériaux, le son de blé peut être un précurseur alternatif intéressent afin d'adsorbé un métal lourd toxique tel que le cadmium.
Mots clés: piles à cadmium, adsorption, son de blé, précurseur alternatif

Corresponding Email: kh_charif@yahoo.fr

O-13

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Preparation and characterization of offertite zeolites exchanged with copper, silver, and zinc for antibacterial applications

Ilyes BOULEDJOUAD [a], Djamel DARI [a], Farid BENNABI [b], Fatiha Djafri [a]

[a] Materials Chemistry Laboratory, Department of Chemistry, University of Oran 1 Ahmed Ben Bella, B.P. 1524 El Mnaouer, 31000 Oran, Algeria

[b]Laboratory of Materials Sciences and Applications (LSMA), University of Ain Temouchent Belhadj Bouchaib, Faculty of Sciences and Technology, Algeria

Abstract:

Zeolites are crystalline microporous aluminosilicates consisting of SiO_4 and AlO_4 Tetrahedra. The substitution of a Si^{4+} ion by an Al^{3+} ion in the framework of a zeolite creates a negative charge that must be compensated for by a cation (alkali cation, alkaline-earth cation, ammonium (NH_4^+), quaternary ammonium (R_4N^+)) [1-3]. This phenomenon is at the origin of a zeolite's ion exchange properties.

In this study, we investigated the hydrothermal synthesis of offretite zeolite using various organic structure directing agents (OSDA), including tetramethylammonium hydroxide (TMAOH), tetraethylammonium hydroxide (TEAOH), 1,6-diaminohexane (DAH), trimethylamine (TrMA), and dimethylamine (DMA). Different techniques have been used for the structural and textural characterization of our solids: X-ray diffraction (XRD), scanning electron microscopy (SEM), energy dispersive X-ray spectrometry (EDX), and thermal analysis (TGA-DTA). TMAOH proved to be the best template for obtaining pure offretite free from any impurities. Subsequently, the prepared offretites were ion-exchanged with Ag^+,

Zn^{2+}, and Cu^{2+} ions to evaluate their antibacterial properties. The results obtained were remarkable, demonstrating significant activity against the bacterial strains tested.

Key words: Zeolite, hydrothermal synthesis,organic structure directing agents, characterization, antibacterial activity.

Corresponding Email:
i.bouledjouad@gmail.com

References

[1] D.W. Breck, Zeolite Molecular Sieves: Structure, Chemistry, and Use, vol. 4, Wiley, , New York, 1973.

[2] C. Baerlocher, L.B. McCusker, D.H. Olson, Atlas of Zeolite Framework Types, Elsevier, 2007.

[3] R. Tekin, N. Bac, J. Warzywoda, A. Sacco Jr., J. Cryst. Growth 411 (2015) 45-48.

O-14

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Title: **The role of intrinsic point defects on the production of green hydrogen fuel on the Cu_2WS4 single-layer: ab initio calculation**

Tarik Ouahrani[a], Reda Boufatah, Chewki Ougherb[a], Daniel Errandonea[c]

[a]École supérieure en sciences appliquées, ESSA-Tlemcen, BB 165 RP Bel Horizon, Tlemcen 13000, Algeria
[b] Laboratoire de Physique Théorique, Université de Tlemcen, Tlemcen 13000, Algeria
[c]Instituto de Ciencia de Materiales, Matter at High Pressure (MALTA) Consolider Team, Departamento de Física Aplicada, Universidad de Valencia, Edificio de Investigación, C/Dr. Moliner 50, Burjassot, 46100 Valencia, Spain

Abstract:

The difficulties brought forth by climate change necessitate ongoing advancements and material discovery for the creation of green hydrogen. Using catalytic hydrogen evolution reactions, point defect engineering is a promising approach for green hydrogen production. In this work, we study the catalytic activation of Cu2WS4 single layers by examining the effect of anionic and cationic vacancy point defects and the active site composition. Density-functional theory simulations have been used to extensively analyze the stability of both the pristine and charged point defect structures of Cu_2WS_4. The Cu vacancy is the one that is most advantageous chemically, according to a thorough examination of the formation enthalpy. On the other hand, the estimated adsorption energy suggests that the hydrogen evolution mechanism is somewhat accelerated by the existence of these vacancies. In contrast, the formation of an S vacancy considerably magnifies the same reaction in Cu_2WS_4 single layers.

Key words: .hydrogen production, Tafel- Volmer reactions, sulfur vacancy, energy adsorption

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Valorization of date seeds for the formulation of an activated carbon with a purifying effect on industrial oils

Belmimoun Asmaa[a],Soltani mohammed El Ghazali[b],Berrami Mohammed[b],Hantour Razika[c]et Chikhaoui Fatima[c]

[a] Bioconversion laboratory microbiology engineering and health safety,University of Mascara ,Algeria
[b] Master's degree in Ecology and environment,university of Mascara,Algeria
[c] Master's degree in Nutrition and dietetics,University of Mascara,Algeria

Abstract:

In this study, we focused on the valorization of date palm (*Phoenix dactylifera L*) seeds in various fields such as agri-food and therapy. Firstly, we examined the physicochemical characteristics of date pits. The results revealed that the pits have characteristics such as 5.83% moisture content, a pH of 6.43, titratable acidity of 1.18, ash content of 0.92, as well as high dry matter content (94.16%). Furthermore, date pits contain proteins (2.89%), and fats (6.05%).

Next, our work involves producing powdered activated carbon from these date seeds, which is capable of absorbing pollutants present in industrial wastewater. Based on the results obtained, our activated carbon can reduce hydrocarbon levels from 19 mg/l to 5.3 mg/l after 2 hours of contact. It also achieves results of 12 mg/l to 5.3 mg/l for suspended solids (SS) and 193 mg/l to 167 mg/l for chemical oxygen demand (COD). The biochemical oxygen demand (BOD5) decreases from 75.2 mg/l to 0 mg/l at a pH of 6 in sample site 1 (before the biological basin), and the pH drops to 3.6; COD decreases from 100 mg/l to 88 mg/l, and hydrocarbon decreases from 1.2 mg/l to 0 mg/l after 1 hour of contact with the activated carbon. In sample site 2 (after the biological basin), BOD5 decreases from 64 mg/l to 35 mg/l. All the results are satisfactory and within international standards.

Finally, we conducted tests on the decolorization of industrial wastewater, obtaining very good results. We found that our activated carbon can be reused once after washing and is ready to be used in industries with its results and renewable raw materials.

Key words: Date seeds, Bio-activated carbon, valorization, industrial effluents, adsorption

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Characterisation of leachates from the Sidi Bel Abbes landfill site and their treatment by adsorption on Hydroxyapatite

Ramdani nadia[a], Chiali charif khadidja[b], Bouazef mokhtar[c]

[a]Ramdani' Energies and Process Engineering Department ,Faculty of Technology, Djillali Liabes University of Sidi bel abbes, Algeria.
[b]Chiali, Environmental Sciences Department, Faculty of Life and Natural Sciences , Djillali Liabes University of Sidi Bel Abbes, Algeria.
[c]Bounazef, Mechanical Engineering Department ,Faculty of Technology, Djillali Liabes University of Sidi bel abbes, Algeria.

Abstract:

Sanitary landfilling is a technique for the disposal of inexpensive and well-established waste management system, applied worldwide. However, it also generates leachates, which are complex and highly polluted wastewaters, they contain a wide variety of recalcitrant compound that make them quite difficult to treat by conventional methods. The aim of this work is to prepare a wet hepatic using a precipitation method from calcium carbonate; characterisation and application on waste leaching. This is due, in order to evaluate the adsorption efficacy and the removal of pollutant load. The treatment by precipitation will make it possible to obtain an effect leading to the reduction of organic and mineral pollutants to reduce toxic nuisances and the protection of the environment.

Key words: Environment, Leachate, Treatment, Hydroxyapatite, Organic pollutants.

Corresponding Email: nadia_ramdani@ymail.com

References

[1] Baun, A., Ledin, A., Reitzel, L. A., Bjerg, P.L., Christensen T. H. (2004), Xenobiotic organic compounds in leachates from ten Danish MSW Xenobiotic organic compounds in leachates from ten Danish MSW landfills chemical analysis and toxicity tests, Water Res, 38, 3845– 3858.

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Structural, electronic and optical properties of perovskites compounds XBS3 (X: Cs,In).

Mahdjoub kheireddine zoubir[a]

[a] Laboratory Physico-Chemestry of Advanced Materials,University of Djillali Liabes;BP89,22000,Sidi Bel Abbés,Algeria

Abstract:

We present the results of our study on the ground state and pressure-induced changes in structural, electronic, and optical properties of XBS3 (X: Cs, In) using density functional theory in the Wien2k code. The lattice parameters of the ground state were found to be consistent with experimental and theoretical findings. Pressure was applied in increments of 3 GPa up to 15 GPa to observe its effects on XBS3 (X: Cs, In). Although the lattice constant and bond length decreased with increasing pressure, the cubic structure of XBS3 (X: Cs, In) remained unchanged. The band structure analysis revealed a direct band gap of 0.80 eV, which decreased to 0.62 eV at 15 GPa. Optical properties within the energy range of 0-13.5 eV indicated a shift towards higher energies under pressure. The direct band gap and strong absorption capabilities of XBS3 (X: Cs, In) in the ultraviolet and visible range suggest its potential for use in optoelectronic devices operating within these wavelengths.

Key words: Density, Functional Theory, electronic properties, optical properties, wien2k code, direct band gap.

Corresponding Email: mahdjoub.kheireddine.zoubir@gmail.com

O-18

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

WATER TREATMENT WITH COMPOSITE BEADS (CALCIUM-ALGINATE/ACTIVATED CARBON)

Mokhtaria Dehar[a,b], Moulkheir Ayat [c,d] ; Sofiane Khanoussi [a,e] ; Fatima Zohra Sebba[b]

[a]Department of Exact Sciences, Oran's Higher Teachers College AMMOUR Ahmed, 02 avenue des martyrs, Oran, Algeria.
[b]Laboratory of Macromolecular Physical Chemistry, Department of Chemistry, University of Oran1 Ahmed Ben Bella, BP 1524 EL-M'Naouer Oran, Algeria.
[c]Department of Chemistry, Faculty of Sciences, Dr Moulay Taher University, BP 138 City, 20000 Nasr, Saida, Algeria.
[d]Laboratory of Polymer Chemistry, Department of Chemistry, Faculty of Exact and Applied Sciences, University of Oran 1 Ahmed Ben Bella, BP 1524 El'Menouer. Oran, Algeria.
[e]Laboratoire de Synthèse Organique Appliquée, Département de Chimie, Faculté des Sciences Exactes et Appliquées, University of Oran1 Ahmed Ben Bella, BP 1524 EL-M'Naouer Oran, Algeria.

Abstract:

Water constitutes the essential element for all existence and fundamental for the economy of humanity. Unfortunately, this source is affected by all types of pollution such as: natural, industrial and chemical pollution [1]. The application of the adsorption phenomenon has been widely used in several works using adsorbent materials in this case: activated carbon, alginate, clay, etc [2-4]. Activated carbon is one of the most commonly used biomaterials to purify water and liquids [5]. In this work, we carried out the preparation of a biomaterial with the aim of preserving the environment. The biomaterial is a composite formed by encapsulation of sodium alginate from powdered activated carbon in the form of solid spheres. These composite beads have been perfectly characterized and they have been used in the elimination of a food additive Sodium Ascorbate (SA). These composite gel beads have been studied using several parameters such as: mass effect, effect of time and concentration, kinetic study, adsorption isotherms and effect of temperature, in terms of their adsorption

capacity on the food additive Sodium Ascorbate in aqueous solution. These parameters were evaluated using UV-visible spectroscopy. The maximum retention of SA is for an average time of 3 hours with a very small quantity of adsorbent m= 0.25g, and the sorption mechanism is described by pseudo-first-order. The adsorption isotherm is compatible with Langmuir's theoretical adsorption model. The thermodynamic parameters showed that the adsorption process is spontaneous, disordered and endothermic ($\Delta G < 0$, $\Delta S > 0$, $\Delta H > 0$). The process thus obtained is of a physical nature (physisorption).

Key words: Activated carbon, Adsorption, Alginate, Composite beads, Sodium ascorbate.

Corresponding Email: deharmokhtaria@yahoo.fr

References

1- Peng, J., Song, Y., Yuan, P., Xiao, S., Han, L. An novel identification method of the environmental risk sources for surface water pollution accidents in chemical industrial parks. Journal of Environmental sciences, 25(7), 1441-1449, **2013**.

2- Quesada, H.B.; de Araújo, T.P., Vareschini D.T., de Barros, M.A.S.D., Gomes, R.G.; Bergamasco, R. Chitosan, alginate and other macromolecules as activated carbon immobilizing agents: A review on composite adsorbents for the removal of water contaminants. Int. J. Biol. Macromol, 1640, 2535–2549, **2020**.

3- Ullah, N., Zarshad, A., Ullah, S., Khan, A.S., Adalat, B., *et al.* Synthesis of activated carbon-surfactant modified montmorillonite clay-alginate composite membrane for methylene blue adsorption. *Chemosphere*, 309, 136623, **2022**.

4- Ai, L., Ming Li, and Long Li. Adsorption of methylene blue from aqueous solution with activated carbon/cobalt ferrite/alginate composite beads: kinetics, isotherms, and thermodynamics. *Journal of Chemical & Engineering Data* 56.8: 3475-3483, **2011.**

5- Caturla, F., Molina-Sabio, M., and Rodriguez-Reinoso, F. Preparation of activated carbon by chemical activation with ZnCl2. *Carbon*, 29, 7, 999-1007, **1991**.

O-19

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Title: **Impact of various doping elements on the structural and electronic properties of quaternary chalcogenides CZTS : DFT study**

Mohamed Amine Chenafi [a], Abdesselam Boucif [b], Kamel Demmouche [c]

[a]Mohamed Amine Chenafi ' Faculty of sciences & technologies, University of Ain Temouchent, BP 284, 46000, Algeria,Magnetic materials laboratory ,University of Djillali Liabes, BP 89, Sidi-Bel-Abbes, 22000, Algeria,

[b] Abdesselam Boucif' Faculty of sciences & technologies, University of Ain Temouchent, BP 284, 46000, Algeria,Magnetic materials laboratory ,University of Djillali Liabes, BP 89, Sidi-Bel-Abbes, 22000, Algeria,

[c] Kamel Demmouche ' Faculty of sciences & technologies, University of Ain Temouchent, BP 284, 46000, Algeria , Magnetic materials laboratory ,University of Djillali Liabes, BP 89, Sidi-Bel-Abbes, 22000

Abstract:

Experimental studies identify the formation of intrinsic point defects near the front interface (e.g., Fermi level pinning due to Cu-Zn antisite defects) and within bulk (bulk recombination due to deep defects) as the key culprits behind the undesirable performance of solar cells. In order to suppress these defects, understanding its formation mechanism during the synthesis of kesterite phase is essential to the ultimate optimization for the fabrication process.

Thus, it is necessary to find an alternative of the Zn element to reduce the disordered cations. In the present work, we substitute Zn atoms in CZTS with Cr and Cd atoms and study the effects of concentration-varied substitution on the band structure and stability of the doped material using the functional theory of density (DFT) and supercell techniques.

Key words: CZTS , doping , SCAN, first principles calculations.

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Numerical Simulation of Tunnel Junction in Multi-Junction Solar Cells Using Silvaco Atlas Software.

DENNAI Benmoussa[a], BOUKAIS Merieme[b], ATOUANI Toufik[a],

[a] Matter Sciences Department, Faculty of Exact Sciences, University Tahri Mohammed Béchar Algeria
[b] Higher School in Electrical and Energy Engineering of Oran, Algeria

Abstract:

In this paper, we present a study and analysis of tunnel junction in Multi-junction solar cell thickness and doping for the tunnel junction. The effect of the tunnel junction layer's in tandem solar cell on it photovoltaic parameters are described. The first step in this simulation is to study the effect of tunnel junction (GaAs) thickness (from 16nm to 32nm) by keeping its doping constant (N_D=N_A= $3x10^{19}$ cm^{-3}). In the second step the doping is varied and the optimum thickness obtained previously is kept constant. The maximum conversion efficiency of 23.42 % is obtained for 16nm and $7x10^{19}$ cm^{-3} for the optimal thickness and doping concentration respectively, these results are obtained under standard conditions test (SCT, AM1.5G, 0.1 W/cm^2, 300 K and 1sun).

Key words*:* tunnel junction, Multi-junction, the optimal thickness, maximum conversion, doping concentration.

Corresponding Email: dennai.benmoussa@univ-bechar.dz

References

[1] Handbook of photovoltaic science and engineering, ed. by Antonio Luque and Steven Hegedus, 2003.
[2] Silvaco ATLAS (vol I&II) user's manual, Silvaco International.
[3] A. Sharenko, Optimization of tunnel diodes in multi-junction solar cells, the 2009 NNIN REU research accomplishments, Electronics (2009) 60–61.

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Transport sélectif des ions métalliques Cd(II) par D2EHPA dans une cellule microfluidique

Lynda Mitiche[a], Amar Sahmoune[a]

[a] *Département de chimie, Faculté des Sciences, Laboratoire de Physique et Chimie des Matériaux LPCM, Université Mouloud Mammeri Tizi-Ouzou.*

Résumé:

Ce travail porte sur l'étude des performances d'une membrane polymère à inclusion à extraire sélectivement le cadmium (II) dans une cellule microfluidique à multicanaux par l'extractant l'acide di-(2-ethylhexyl) phosphorique (D2EHPA). Ce ligand-transporteur de pKa= 3,5 choisi est une molécule de la famille des organophosphorés très bon complexant de cations métalliques polluants présents dans les rejets industriels. Pour cela, nous avons élaboré une membrane MPI à partir du tri acétate de cellulose (TAC) comme support polymérique et D2EHPA comme transporteur et d'un plastifiant 2- nitrophenyl octyl ether (2-NPOE) que nous avons caractérisée par les techniques physico-chimiques. Les résultats de la caractérisation ont montré que les différents constituants cristallisent dans la matrice de la membrane en conservant leur structure sans interactions chimiques entre eux. L'équilibre d'extraction des ions métalliques divalents par le D2EHPA noté HR est décrit par l'équation suivante:

$$M^{2+}_{aq} + 2\,(HR)_{2org} \Leftrightarrow MR_2(HR)_{2org} + 2\,H^{+}_{aq}$$

Les résultats des expériences de transport des trois cations métalliques obtenus ont montré que les performances des membranes sont satisfaisantes dans le dispositif microfluidique. Il a été observé qu'une faible augmentation de la concentration en D2EHPA (de 2,5% à 10%) permet d'augmenter le taux de transport du cadmium de 45% à 99% et que le D2EHPA présente une forte affinité et sélectivité pour le cadmium dont le transport est quasi-quantitatif. Cette étude a montré également que le système microfluidique développé permet de séparer les ions Cd^{2+}/Zn^{2+} et les ions Cd^{2+}/Ni^{2+} avec une assez bonne efficacité.

Ce travail ouvre une perspective plus grande pour l'extraction microfluidique d'ions métalliques par membranes d'affinité.

Mots clés:

Membrane polymère à inclusion, cellule microfluidique, cadmium, D2EHPA.

Corresponding Email: lynda.mitiche@ummto.dz

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Highly Potent Antibacterial Copper-Based MOFs/Na-Alginate Composite Beads

Fatima Zohra Zeggai,[a, b] Masika Bradai,[a] Massillia Ait Radi,[a] Noureddine Karkachi, [c] and Rachid Meghabar [a]

a. Laboratoire de chimie des polymères (LCP), Département de chimie. Université d'Oran 1 Ahmed Benbella, BP 1524, El-Mnaouer, 31000 Oran, Algeria

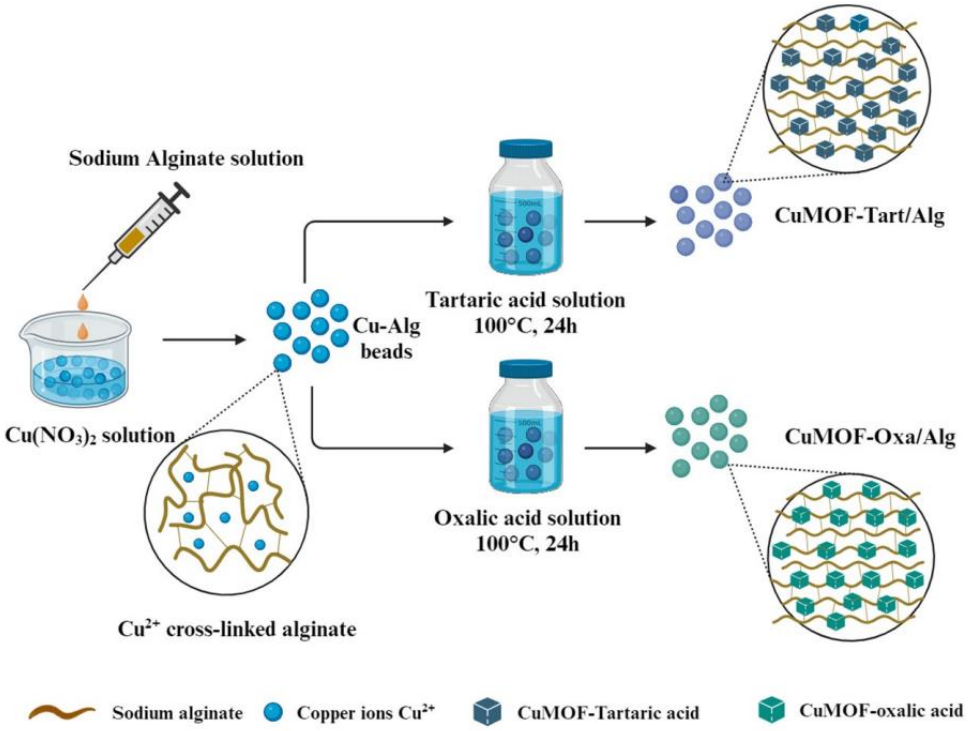
b. Centre de Recherche Scientifique et Technique en Analyses PhysicoChimiques (CRAPC), BP 10 384, siège ex-Pasna Zone industrielle, Bou-Ismail CP, 42004 Tipaza, Algeria

c. Laboratoire de Microbiologie Appliquée (LMA). Département de biologie. Université Oran1 Ahmed Benbella, BP 1524, El-Mnaouer, 31000 Oran, Algeria.

Abstract:

The present study reports an environmentally friendly in-situ synthesis of novel antibacterial copper-based MOFs within the hydrogel network of sodium alginate. Two different copperbased MOF/sodium alginate composite beads were prepared via the post-treatment of copper-ion-crosslinked alginate hydrogels with two different ligand solutions, namely, tartaric acid and oxalic acid, at 100°C for 24 h. The structural, thermal, and morphological properties of the prepared samples were investigated using Fourier transform infrared spectroscopy (FTIR), Xray diffraction (XRD), thermogravimetric analysis (TGA), and scanning electron microscopy (SEM), and their antibacterial activities against gram-positive (Staphylococcus aureus and Bacillus) and gram-negative (Escherichia coli and Pseudomonas aeruginosa) strains were examined using the conventional disc diffusion method. The results demonstrated the success of the in-situ synthesis of two distinct copper-based MOFs with FTIR spectra, confirming the existence of characteristic bands of the ligands complexed to the sodium

alginate matrix. Moreover, the XRD diffractograms revealed the formation of two distinct crystalline structures with well-defined morphologies observed in the SEM images. In addition, thermal analysis showed that the prepared composite beads had enhanced thermal stability compared to the copper-ion-crosslinked alginate beads. Antibacterial testing revealed the strong capacity of the copperbased MOFs/sodium alginate composite beads to deactivate the growth of all the bacterial strains used, with a minimum inhibition zone of 23 mm, which highlights the potential of the synthesized materials as highly potent antibacterial agents.



Graphical Abstract

Key words: copper-based MOFs, in-situ synthesis, sodium alginate, hydrogel network, tartaric acid, oxalic acid, antibacterial activity.

Corresponding Email:
___zeggai.fatimazohra@gmail.com_____

References

[1] .....

[2] .....

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Title: Structural Damage Identification in composite beam using modal data and metaheuristic

M-A Lounis[a], A Kahouadji[a], A Behtani[a], S Tiachacht[a] and M Slimani[a]

[a] Laboratory of Mechanics, Structure and Energetics (LMSE), Mouloud Mammeri University of Tizi-Ouzou, B.P.N°17 RP, 15000, Algeria.

Abstract:

Even if seen as well made, every structure, machine, and tool certainly have visible or invisible defects that vary in location, number, and size. Different aspects such as, machining processes, wear and impact generate them. In recent years, most works in structural dynamics have aimed at evaluating and reconciling numerical models and experimental structures. The different damage detection and quantification methods give an overview of defects and their magnitudes. The work consists in first time to detect and determine the modal and frequency difference between the undamaged structure and the damaged structure by the FRF method, then exploit and use these results in different optimization algorithms to detect and quantify this damage. This work mainly aims to test three previously published optimization algorithms, which are the African Vulture Optimization Algorithm (AVOA), the Salp Swarm Algorithm (SSA), and the Whale optimization algorithm (WOA). These algorithms are tested on a multilayer composite structure to verify their effectiveness in detecting and quantifying structural damage. Comparing these three methods will be handy for choosing the appropriate method.

Key words: . Damage quantification; Optimization algorithms; Composite structures; AVOA; SSA; WOA.

Corresponding Tel.: +213 676 66 95 88; E-mail address: mohand-amokrane.lounis@ummto.dz

_____

References

[1] A. Kahouadji, S. Tiachacht, M. Slimani, A. Behtani, S. Khatir, and B. Benaissa, "Vibration-Based Damage Assessment in Truss Structures Using Local Frequency Change Ratio Indicator Combined with Metaheuristic Optimization Algorithms," in International Conference of Steel and Composite for Engineering Structures, 2022: Springer, pp. 171-185.

[2] H. Hwang and C. Kim, "Damage detection in structures using a few frequency response measurements," Journal of sound and vibration, vol. 270, no. 1-2, pp. 1-14, 2004.

[3] S. Tiachacht, A. Bouazzouni, S. Khatir, M. A. Wahab, A. Behtani, and R. Capozucca, "Damage assessment in structures using combination of a modified Cornwell indicator and genetic algorithm," Engineering Structures, vol. 177, pp. 421-430, 2018.

[4] S. Khatir, S. Tiachacht, C. Le Thanh, T. Khatir, R. Capozucca, and M. Abdel Wahab, "Damage Detection in Laminated Composite Plates Based on Local Frequency Change Ratio Indicator," in Proceedings of the 13th International Conference on Damage Assessment of Structures, Singapore, M. A. Wahab, Ed., 2020// 2020: Springer Singapore, pp. 887-898.

[5] G. F. Gomes, S. S. da Cunha, and A. C. Ancelotti, "A sunflower optimization (SFO) algorithm applied to damage identification on laminated composite plates," Engineering with Computers, vol. 35, no. 2, pp. 619-626, 2019/04/01 2019, doi: 10.1007/s00366-018-0620-8.

[6] S. Tiachacht, A. Bouazzouni, S. Khatir, M. Abdel Wahab, A. Behtani, and R. Capozucca, "Damage assessment in structures using combination of a modified Cornwell indicator and genetic algorithm," Engineering Structures, vol. 177, pp. 421-430, 2018/12/15/ 2018, doi: https://doi.org/10.1016/j.engstruct.2018.09.070.

[7] D. Gürses, P. Mehta, S. M. Sait, and A. R. Yildiz, "African vultures optimization algorithm for optimization of shell and tube heat exchangers," Materials Testing, vol. 64, no. 8, pp. 1234-1241, 2022.

[8] S. Mirjalili, A. H. Gandomi, S. Z. Mirjalili, S. Saremi, H. Faris, and S. M. Mirjalili, "Salp Swarm Algorithm: A bio-inspired optimizer for engineering design problems," Advances in engineering software, vol. 114, pp. 163-191, 2017.

[9] S. Mirjalili and A. Lewis, "The whale optimization algorithm," Advances in engineering software, vol. 95, pp. 51-67, 2016.

[10] D. Dinh-Cong, H. Dang-Trung, and T. Nguyen-Thoi, "An efficient approach for optimal sensor placement and damage identification in laminated composite structures," Advances in Engineering Software, vol. 119, pp. 48-59, 2018.

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Experimental study of structural inhomogeneities in Heusler materials

AMERI Ibhraim[a], BLAHA Lamia Farah[a], KHATIR Radja[b]

[a]University Djillali Liabbes Sidi Bel Abbes . Physico-Chemiistry Laboratory of Advanced Materials
[b] Laboratory of Electrical Engineering and Materials (LGEM), Oran, 31000, Algeria

Abstract:

Our current work investigates the structural properties of Heusler materials prepared by fusion growth, using various thermal regimes. We studied the compositional behavior of the polycrystalline material obtained from stoichiometric and respectively non-stoichiometric fusions. X-ray diffraction and scanning electron microscopy complement each other in the characterization of the phases occurring in the samples. The synthesis of Heusler materials from an initially stoichiometric mixture associated with a heat treatment presenting plateaus gives the best results.

Key words: fusion growth , X-ray , stoichiometric.

Corresponding Email: ameriibrahim22@gmail.com

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

EXTRAITS DE PLANTES COMME INHIBITEURS DE CORROSION VERTS POUR LA PROTECTION DES METAUX

FERHAT Mahmoud[a], GAOUI Halima[b]

[a,b] Material science department; laboratory of mechanics/University of Laghouat, Algeria

Abstract:

The use of green corrosion inhibitors, which reduce corrosion rates to an acceptable level with a low environmental impact, is one of the most important new approaches to controlling corrosion in modern society. The emergence of "green" chemistry has led to the use of plant extracts and fruit wastes that have proven to be good corrosion inhibitors. From an environmental point of view, this area of research is undergoing significant developments. As a result of growing environmental awareness, corrosion inhibitors are now subject to strict restrictions and regulations imposed by the environmental authorities of several countries, in particular Algeria. According to these requirements, these chemicals must be acceptable and safe for the environment. With this in mind, intensive research has been carried out in recent years to develop green corrosion inhibitors from plant extracts. They must be readily available, inexpensive, biodegradable and safe. Oils and plant extracts have become a source of inhibitors that provide high environmental efficacy at a lower cost. These types of inhibitors do not contain heavy metals or toxic compounds and are biodegradable. They are promising alternatives to hazardous conventional corrosion inhibitors. The purpose of this presentation is to briefly summarise a compilation of recent leading articles on the use of plant extracts as sustainable and green corrosion inhibitors. In addition, we will present the advantages and disadvantages of using these substances to protect metals.

Keywords: Corrosion protection, Corrosion inhibitor, Green chemistry, Plant extracts Phytochemicals.

Corresponding Email: m.ferhat@lagh-univ.dz

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Optimizing Performance of $KSnI_3$-Based Perovskite Solar Cells with Tin (Sn) using SCAPS Software

Badiaa BACHIRI[a,b], Khadidja RAHMOUN[a,b]

[a]*Department of physics, Faculty of sciences, University of Tlemcen AbouBekr Belkaid, Tlemcen Algeria*
[b]*Unit of Research on Materials and Renewable Energies, URMER, Tlemcen, Algeria*

Abstract:

This research paper studies perovskite solar cells using tin (Sn) as the base material and employing SCAPS software for analysis, focusing on the absorbing KSnI3 perovskite layer[1]. The study reveals key results including fill factor (FF) of 88.27%, power conversion efficiency (PCE) of 15.51%, open circuit voltage (Voc) of 1.2871 V and a short-circuit current density (Jsc). of 13.653229 mA/cm². Furthermore, the investigation identifies that the optimal thickness of the KSnI3 layer is 1 µm, resulting in a remarkable PCE of 19.4257%. The research also highlights the impact of defect density on performance, showing that an increase in the number of defect sites leads to more traps and recombinations paths, ultimately reducing efficiency. These results highlight the potential of KSnI3 [2]-based perovskite solar cells as viable candidates for high-efficiency photovoltaic applications.

Key words: Perovskite solar cells, $KSnI_3$, Power conversion efficiency, SCAPS 1D

Corresponding Email: bachiribadi3a@gmail.com

References

[1] G. Pindolia, S. M. Shinde, and P. K. Jha, 'Non-leaded, KSnI3 based perovskite solar cell: A DFT study along with SCAPS simulation', *Materials Chemistry and Physics*, vol. 297, p. 127426, Mar. 2023, doi: 10.1016/j.matchemphys.2023.127426.

[2] B. Bachiri and K. Rahmoun, 'Numerical Simulation of Perovskite Solar cell with Porous Silicon layer', p. 6, 2022.

ICMSE'2024

The 3rd edition of the International Conference on Materials Science and Engineering and their impact on the Environment

Fiber Optic Nanotechnology: Shaping the Future of Communication

Samia DRIZ[1], Benattou FASSI[1]

[1]Telecommunications and Digital Signal Processing Laboratory, Faculty of Electrical Engineering, University of Djillali Liabes, Sidi Bel Abbes, Algeria

Abstract:

Fiber optic communication has revolutionized information transmission, forming the backbone of our global infrastructure. However, the insatiable demand for bandwidth and efficiency necessitates continuous advancements. Enter fiber optic nanotechnology, poised to rewrite the future of communication. This transformative approach introduces novel materials like nanowires and rare-earth dopants, opening doors to unprecedented light manipulation. Nanowires, with their ultra-thin structure, guide light with unparalleled precision, minimizing scattering and absorption losses. Nanoparticles dispersed within the fiber matrix tailor the refractive index, leading to improved light confinement and reduced signal attenuation. Beyond mere light propagation, nanotechnology unlocks novel functionalities within optical fibers. Wavelength conversion becomes feasible by exploiting nonlinear optical effects induced by nanoscale structures. This allows the conversion of signals from one wavelength to another, facilitating wavelength division multiplexing and exponentially increasing the overall capacity of communication systems. Moreover, micro/nano-structured fibers offer intricate core designs for manipulating light in unique ways, leading to enhanced signal control, dispersion management, and nonlinearity suppression. Additionally, surface plasmon resonance (SPR), utilizing the interaction between light and metal nanoparticles on the fiber surface, enables real-time sensing of various parameters like temperature, pressure, and chemical composition. These advancements promise to revolutionize communication by significantly increasing bandwidth and data capacity, integrating security features and signal processing within the fiber itself, and enabling real-time data collection through fiber optic sensors for diverse applications. This integration of nanotechnology into the core of fiber optics paves the way for next-generation communication networks with unprecedented efficiency, reliability, and diverse functionalities, fundamentally transforming how we transmit and process information.

Keywords: Nanotechnology, Optical fibers, Communication networks, Fiber optic communication.

ICMSE'2024

The 3rd edition of the International Conference on Materials Science and Engineering and their impact on the environment

PbS Colloidal Quantum Dot-Based Photodetectors: A Promising Approach for Enhanced Performance in Visible Light Communication Systems

Benattou FASSI[1], Samia DRIZ[1]

[1]Telecommunications and Digital Signal Processing Laboratory, Faculty of Electrical Engineering, University of Djillali Liabes, Sidi Bel Abbes, Algeria

Abstract:

Recent advancements in optical communication technologies have spurred the development of Next-Generation (NG) systems capable of delivering higher data rates, improved spectral efficiency, and extended transmission distances. In response to the continually escalating and ambitious requirements of contemporary connectivity, researchers are exploring innovative solutions. This encompasses harnessing artificial intelligence algorithms, pioneering novel materials, delving into the potential of quantum communication, and propelling the advancement of fiber optic networks. In this dynamic landscape, the integration of Colloidal Quantum Dot (CQD)--based photodetectors (PDs) into optical frameworks stands out as a pivotal development. Among the plethora of choices available, PbS colloidal quantum dot-based photodetectors have risen as a leading contender, signaling the dawn of a fresh era characterized by enhanced efficiency and performance in data transmission. Their exceptional promise lies in their remarkably high responsivity and seamless compatibility with near-infrared wavelengths, attributes that are poised to redefine the capabilities of optical communication systems. Lead sulfide colloidal quantum dots exhibit unique optoelectronic properties, including a tunable bandgap (0.6–1.6 eV), meaning their light absorption range can be adjusted, from the visible to the Near-Infrared (NIR) region (200–2500 nm), by controlling their size. This allows them to be tailored for specific applications within the optical spectrum. Furthermore, PbS CQDs can absorb light very efficiently, leading to highly sensitive photodetectors capable of detecting even weak light signals. Also, they can be fabricated using solution-based methods, which are often simpler and less expensive than traditional semiconductor fabrication techniques. These attributes make them attractive for photo-detection applications, where sensitivity, spectral selectivity, and cost-effectiveness are critical factors. This research explores the potential of PbS colloidal QD-based PD to improve the performance of Visible Light Communication (VLC) systems compared to the conventional one, emphasizing key performance metrics such as Q-Factor and Bit Error Rate (BER). Utilizing advanced simulation tools within OptiSystem software, we comprehensively assess

the integration of this novel photodetector within the VLC system, enabling a thorough analysis of its impact on the overall communication performance. The results demonstrate that PbS CQD-based PD offers superior performance metrics compared to conventional detectors. The findings of this study hold significant implications for the development of NG optical systems, particularly in the context of VLC. Integrating PbS CQD-based PDs has the potential to create highly sensitive, compact, and cost-effective VLC systems, offering improvements in coverage, sensitivity, and detectivity. Future research directions include further optimization of device performance, and exploration of new applications enabled by PbS CQD technology. In conclusion, this research paves the way for collaborative efforts between academia, industry, and research institutions to fully realize the potential of PbS CQDs and their transformative impact on VLC and potentially other applications offering a promising pathway toward meeting the growing demands of modern communication networks.

Keywords: Visible Light Communication (VLC), PbS colloidal quantum dot (CQD), Q-Factor, Bit Error Rate (BER)

Corresponding Email: fassi.benattou@univ-sba.dz

References

[1] Fon, R. C., Ndjiongue, A. R., Ouahada, K., & Abu-Mahfouz, A. M. (2023). Fibre optic-VLC versus laser-VLC: A review study. *Photonic Network Communications*, *46*(1), 1-15. https://doi.org/10.1007/s11107-023-00997-z

[2] Zhou, H., Zhang, M., & Ren, X. (2023). Design and implementation of wireless optical access system for VLC-IoT networks. *Journal of Lightwave Technology*, *41*(8), 2369-2380. 10.1109/JLT.2023.3234990

[3] Vafaie, M., Fan, J. Z., Najarian, A. M., Ouellette, O., Sagar, L. K., Bertens, K., and all. (2021). Colloidal quantum dot photodetectors with 10-ns response time and 80% quantum efficiency at 1,550 nm. *Matter*, *4*(3), 1042-1053. https://doi.org/10.1016/j.matt.2020.12.017

[4] Gong, W., Wang, P., Deng, W., Li, J., Li, W., Li, J. et all. (2023). Ultrahigh detectivity from multi-interfaces engineered near-infrared colloidal quantum dot photodetectors. *IEEE Transactions on Electron Devices*, *70*(7), 3668 – 3674. 10.1109/TED.2023.3276730

[5] Huang, W., Wang, S., Gong, H., Tian, J., Peng, J., & Cao, J. (2023). Size tunable and controllable synthesis of PbS quantum dots for broadband photoelectric response. *Optical Materials*, *142*, 113977. https://doi.org/10.1016/j.optmat.2023.113977

[6] Tang, H., Zhong, J., Chen, W., Shi, K., Mei, G., Zhang and all. (2019). Lead sulfide quantum dot photodetector with enhanced responsivity through a two-step ligand-exchange method. *ACS applied nano materials*, *2*(10), 6135-6143. 10.1021/acsanm.9b00889

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Mechanical Characterization of a biocomposite based on polypropylene reinforced with oyster shell particles

Yerou Amine[1], Benaichouba Zahira[1]*, Bel Abbes Bachir Bouiadjra[2] , Bouziane Mohamed Mokhtar[1,2], Salem Mokadem[2] , Bouregba Rachid[1]

[1] Department of Mechanical Engineering , Mustapha Stambouli university of Mascara, Algeria
[2] LMPM, Department of Mechanical Engineering, University of Sidi Bel Abbes, *e-mail : amine.yerou@univ-mascara.dz

Abstract

The biocomposite materials are fabricated by polymers reinforced with natural fibers or natural particles as fillers. Various techniques are used to prepare these biocomposites among which we can mention: molding, intercalation , laser printing, solvent casting, filament winding, fusion mixing ... Seashells represent an abundant source that can be used as a filler for thermoplastic polymers because these shells present a fairly good thermal stability compared to other fillers. They are suitable to be ground into chips or particles. The main element in the composition of seashell is calcium carbonate (CaCO3). In this study biocomposite based on polypropylene (PP) filled with oyster shell participles is characterised with different mechanical tests: tensile test, impact test and micro hardness test. Different proportions of the reinforcement in the biocomposite were used 0%, 10% and 30%. The average size of the oyster shell particles is 200 µm. The samples used in the mechanical tests were made by injection molding to ensure a good dispersion of the filler particles in the PP. The tensile test results show that the oyster shell particles improve the rigidity of the PP and its mechanical strength. The ductility of the PP is reduced by the reinforcement. On the other hand, the impact strength of the PP is highly increased by the bio-particles. These particles also increase the average micro-hardness of the polypropylene.

KEY-WORDS : polypropylene, Oyster shell, Tensile test, Impact test, Micor hardness.

O-30

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Photocatalytic hydrogen production over MFe_2O_4 (M=Ca, Cu) nano-spinel powders under visible light irradiation.

Hamza MEDJADJI [a*], Ali BOULAHOUACHE [a,b], Khaled DERKAOUI[c], S. E. BERRBAH[d] Mohamed TRARI[e], Nachida BENSEMMANE[a],Nassima SALHI [a,b]

[a*] Laboratoire LCPMM, Faculté des Sciences, Université BLIDA1, B.P 270, Route de Soumaa, BLIDA, Algérie.
[b] Laboratoire de Chimie du Gaz Naturel, Faculté de Chimie, USTHB, BP32, El-Alia, 16111 Bab Ezzouar, Alger, Algérie.
[c]Research Center On Semiconductors Technology for Energetic, CRTSE-TESE - 02, Bd. Dr. Frantz Fanon, 7 Merveilles, Box 140, 16038 Algiers, Algeria.
[d]Laboratory of Electrochemistry-Corrosion Metallurgy and Inorganic Chemistry, Faculty of Chemistry (USTHB), BP 32, 16111 Algiers, Algeria
[e]Laboratoire de Stockage et valorization de l'énergie renouvelable, Faculté de Chimie, USTHB, BP32, El-Alia, 16111 Bab Ezzouar, Alger, Algérie.

Abstract:

Hydrogen produced from renewable energy, such as solar, is known as green hydrogen [1]. Hydrogen production from water using semiconductors such as photocatalysts has attracted wide attention due to its potential application for solving the energy crisis and environmental pollution [2]. MF2O4 spinel ferrites type have shown broad interest in diverse energy conversion processes, including fuel cells and photo electrocatalytic water splitting [3].

Nano-spinels MFe_2O_4 (M= Ca, Cu), were prepared by nitrate method as photo-catalysts. The physical and optical properties were analyzed by thermal gravimetric analysis (TGA-DT), X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR), UV-visible spectroscopy, scanning electron microscopy (SEM-EDX), photoelectron spectroscopy X(XPS), and electrochemical analysis. The photocatalytic performances were evaluated by hydrogen production under visible light irradiation.

XRD analysis sindicated the formation of pure phases at 850°C with an average particle size in the range of 31- 40 nm. SEM images showed heterogeneous grains with irregular shapes in both spinels. EDX elemental analysis determined the presence of (Ca, Fe, and O) in the calcium ferrite and (Cu, Fe, and O) copper ferrite, which confirms the high purity of both

prepared materials. The Mott-Schottky measurement (C−2–E) indicated the p-type behavior for all spinels.

The photocatalytic performance was successfully evaluated for H_2 production. The higher activity is obtained with $CaFe_2O_4$ in Na_2SO_4 electrolyte at pH ~ 7, with an amount of 189 µmol, wherea 84 µmol of hydrogen release on $CuFe_2O_4$ was achieved in basic medium (pH ~ 12), under visible light Irradiation at optimum temperature.

Key words: MFe_2O_4 (M=Ca, Cu), Nitrate route, Synthesis, Hydrogen, Photocatalytic

Corresponding Email:

hamzamedjadji1990@gmail.com

[1]D. Yamashita, K. Tsuno, K. Koike, K. Fujii, S. Wada, and M. Sugiyama, "Distributed control of a user-on-demand renewable-energy power-source system using battery and hydrogen hybrid energy-storage devices," Int. J. Hydrogen Energy, vol. 44, no. 50, pp. 27542–27552, 2019, doi: 0.1016/j.ijhydene.2019.08.234.

[2]H. Lahmar, M. Benamira, F. Z. Akika, and M. Trari, "Reduction of chromium (VI) on the hetero-system CuBi2O4/TiO2 under solar light," J. Phys. Chem. Solids, vol. 110, no. Vi, pp. 254–259, 2017, doi: 10.1016/j.jpcs.2017.06.021.

[3]R. Benrabaa, H. Boukhlouf, S. Barama, E. Bordes-Richard, R. N. Vannier, and A. Barama, "Structural, textural and acid-base properties of nano-sized NiFe 2O 4 spinel catalysts," Catal. Letters, vol. 142, no. 1, pp. 42–49, 2012, doi: 10.1007/s10562-011-0726-8.

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

On the error analysis in NOMA networks: assessing the impact of environmental interference and imperfect SIC

Nour El Houda BOUDA[a], SidAhmed ELAHMAR[b]

[a,b] Telecommunications, Telecommunication and Digital Signal Processing Laboratory, Djillali Liabes University, Algeria.

Abstract:

Future radio access networks (5G and beyond) must handle a diverse set of demanding applications, including ultra-high data rates for immersive virtual reality and high-definition video streaming. In addition, there is a pressing need for ultra-low latency to facilitate real-time applications such as remote surgery and autonomous vehicles. Furthermore, networks must support large connections in order to properly manage the dense ecosystem of the Internet of Things (IoT). Moreover, high mobility support is required to enable continuous connectivity for users in motion. This needs a paradigm change in resource allocation strategies, opening the way for novel solutions such as Non-Orthogonal Multiple Access (NOMA) to address these difficulties and guide to an alternative of conventional wireless communication networks. NOMA thrives on resource sharing, enabled by Superposition Coding (SC) at the transmitter. Multiple users, each with a different power level, occupy the same Resource Block (RB) at the same time, depending on channel circumstances. This resource-efficient approach strategy is based on the ability to correctly separate and decode user signals. To predict NOMA's performance in different environments, channel models have been developed. These models allow researchers to simulate real-world channel behavior and assess the impact of factors like path loss, fading, delay spread, and Doppler shift. These factors are influenced by distance, reflections, scattering, multipath propagation, and user mobility. While these factors in Orthogonal Multiple Access (OMA) systems primarily affect individual users due to their dedicated RBs, NOMA presents a distinct challenge. In NOMA, users share the same RB, making them significantly more susceptible to the channel's interferences. This inherent difference underscores the increased complexity in managing interferences in NOMA compared to OMA, as variations in channel conditions directly affect the decoding process for all users within the shared resource, potentially resulting in suboptimal Successive Interference Cancellation (SIC) performance, where residual interference from stronger users may interfere with the decoding of weaker users' signals.

In many wireless communication scenarios, frequency-selective fading is common. However, when user mobility is introduced, it adds complexity by requiring consideration of doubly selective channels. User mobility means that the positions of the transmitter, receiver, and obstacles in the environment are constantly changing, resulting in a dynamic channel response. This dynamic interplay creates a channel that exhibits both time-dependent variations (due to changing positions) and frequency-dependent variations (due to the inherent frequency selectivity of the environment), making the channel doubly selective. This combination of time-varying and frequency-selective characteristics poses a significant challenge for reliable systems.
This paper investigates the performance of a NOMA system under different doubly selective channel models representing various scenarios and environments. These channel models could include:

- Vehicular A and B: These models represent typical channel conditions experienced by users in vehicular environments, potentially including high speeds and rapid changes in signal strength due to obstacles.
- Pedestrian A and B: These models represent channel conditions encountered by pedestrian users, potentially involving slower speeds but still significant variations in the channel due to the user's movement and surrounding objects.

By simulating NOMA under these diverse scenarios and analyzing the Bit Error Rate (BER) performance, this paper reveals the impact of mobility and the environment on the system's error rate.

Key words: Non-Orthogonal Multiple Access, Doubly selective channels, Imperfect SIC, Interferences, 5G environments.

Corresponding Email: boudanoor@gmail.com.

Acknowledgment: This work was supported by the Directorate General for Scientific Research and Technological Development (DGRSDT).

References

[1] 3GPP, “TSG RAN; study on scenarios and requirements for next generation access technologies; (release 14), Oct. 2016

[2] SALOUS, Sana, TUFVESSON, Fredrik, TURBIC, Kenan, et al. IRACON propagation measurements and channel models for 5G and beyond. ITU Journal: ICT Discoveries, 2019, vol. 2, no 1.

[3] ZHANG, Jianhua. IMT-2020 Channel Model. Wiley 5G Ref: The Essential 5G Reference Online, 2019, p. 1-18.

[4] SHARMA, Priyank, KUMAR, Atul, et BANSAL, Matadeen. Performance analysis of downlink NOMA over η–μ and κ–μ fading channels. IET Communications, 2020, vol. 14, no 3, p. 522-531.

O-32

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Influence of slag powder in rheological behavior of ecofriendly concrete

Hamza SOUALHI[a], Salim SAFIDDINE[b], Akram Salah Eddine BELAIDI[a], El-Hadj KADRI[c], Tien-Tung NGO[c], Lynda Amel CHAABANE[d]

[a] LRGC laboratory, Civil Engineering Department, University of Laghouat – Algeria
[b] LME laboratory, Civil Engineering Department, University of Médéa – Algeria
[c] L2MGC laboratory, Civil Engineering Department, University of CY Cergy-Paris – France
[d] LPCMA laboratory, Civil Engineering Department, Sidi Bel Abbes University, Algeria.

Abstract:

This research examines the rheological characteristics of concrete mixes containing various industrial wastes as partial replacements for cement, aiming to create concrete with reduced environmental impact. A control mix composed solely of Portland cement was compared to other mixes containing combinations of cement and slag with varying replacement rates ranging from 0% to 60%. Using a new concrete rheometer [1], the plastic viscosity and shear yield stress of the concretes were measured at different slump degrees. The results indicate that the type and rate of material substitution influence the rheological properties of low environmental impact concrete. Specifically, an increase in the substitution rate leads to an increase in the plastic viscosity of the concretes made with different types of materials added in this study.

Key words: Rheology, plastic viscosity, yield stress, ecofriendly concrete, slag.

Corresponding Email:

Hamza_s26@yahoo.fr; h.soualhi@lagh-univ.dz

References

[1] H. SOUALHI, E.H. KADRI, T.T. NGO, A. BOUVET, F. CUSSIGH, Z. TAHAR. Design of portable rheometer with new vane geometry to estimate concrete rheological parameters. Journal of Civil Engineering and Management. Volume 23, Issue 3, 347-355, 2017. https://doi.org/10.3846/13923730.2015.1128481

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Traitements Plasmagéne et Plasmacatalytique D'un Colorant Anthraquinonique.

Belkralladi.Halima[a], bouyakoub.Z[b] , Djamaa.Z[b], Ghezzar.M[b], Abdelmalek. .F[c]

Abstract:

es procédés d'oxydation avancés (POA). Reposent sur la formation in situ des radicaux hydroxyles HO° qui possède un pouvoir oxydant très fort et très réactif. « le Glidarc » est un moyen simple et économique générant le même type d'espèces que POA, Il repose sur l'utilisation d'un plasma d'air humide obtenu par décharge électrique à température Modérée et pression atmosphérique. Les espèces génères confèrent au plasma d'air humide des propriétés acidifiantes et oxydantes importantes. Dans notre étude nous avons employé le plasma seul et combiné avec un catalyseur en phase hétéro gène TiO2 (Dégussa P25).

Le traitement plasmagène du colorant AG25 en absence et en présence de TiO2. La décoloration à été suivie par le spectrophotomètre UV/visible et la dégradation par la demande chimique en oxygène (DCO). La décoloration anthraquinonique AG25 a atteint 89% au bout 120 minutes de traitement plasma chimique. L'addition de TiO2 Dégussa P25a permis d'atteindre un taux de 83,7% en seulement 30 minutes de traitement plasmagène. en présence du catalyseur la vitesse de dégradation est 4,2 fois supérieur que traitement sans TiO2.

Key words: colorant, Glidarc, plasma, catalyseur, dégradation.

belkralladihalima@yahoo.fr

halima.belkralladi@univ-sba.dz

O-34

ICMSE'2024

The 3rd edition of the International Conference on Materials Science and Engineering and their impact on the environment

$BaYAlZn_3O_7:Sm^{3+}$-based LEDs Leading the Way in Efficient and Sustainable Visible Light Communication

Halima CHAHED[1], Benattou FASSI[1], Samia DRIZ[1]

[1]Telecommunications and Digital Signal Processing Laboratory, Faculty of Electrical Engineering, University of Djillali Liabes, Sidi Bel Abbes, Algeria

Abstract:

The proliferation of Visible Light Communication (VLC) systems underscores the transformative potential of light as a medium for high-speed data transmission. In the context of modern indoor environments, where connectivity is paramount, VLC systems emerge as indispensable tools for enabling seamless communication. However, the efficacy of VLC hinges upon the utilization of luminescent nanomaterials that not only ensure transmission efficiency but also uphold principles of environmental sustainability. Enter Barium Yttrium Aluminum Zinc Oxide doped with Samarium ($BaYAlZn_3O_7:Sm^{3+}$)-based LEDs, a novel luminescent nanomaterial poised to revolutionize VLC technology. The approach suggests replacing the yellow-phosphor with a new phosphor material that emits orange-red light when excited by Near-UltraViolet (N-UV) radiation, to address the limitations of the traditional method. In this study, we aim to intricate the performance of $BaYAlZn_3O_7:Sm^{3+}$ LEDs within VLC systems, employing advanced simulation techniques within OptiSystem Software to unravel their transmission quality (Q-factor), Bit-Error-Rate (BER) comparatively to conventional LED, Through our comparative analysis, our $BaYAlZn_3O_7:Sm^{3+}$ LED has achieved a transmission distance of 120 meters, all the while maintaining exceptional Q-factor and BER performance. This significant accomplishment surpasses the distance of the traditional material range of 100 meters, affirming the superior capabilities and promising potential of our innovative solution. In addition to transmission efficiency and reliability, this study investigates the environmental impact of $BaYAlZn_3O_7:Sm^{3+}$ LEDs, as well as their significant effects on human beings' health and local plant growth. This study seeks to uncover the transformational potential of $BaYAlZn_3O_7:Sm^{3+}$ LEDs in influencing the future of sustainable communication technology by effectively investigating the delicate interplay between material characteristics, device performance, and environmental consequences. This study provides useful insights into the developing field of VLC research through rigorous analysis and empirical validation, opening the way for increased transmission capacities and encouraging ecological consciousness in optical communication.

ICMSE'2024

The 3rd edition of the International Conference on Materials Science and Engineering and their impact on the environment

Enhancing Next-Generation Optical Systems with $PtSe_2$/ultrathin Al_2O_3/Ge - Based Photodetectors

Rima KEBAILI[1], Samia DRIZ[1], Benattou FASSI[1]

[1]Telecommunications and Digital Signal Processing Laboratory, Faculty of Electrical Engineering, University of Djillali Liabes, Sidi Bel Abbes, Algeria

Abstract:

Recent advancements in optical communication technologies have spurred the development of Next Generation (NG) systems capable of delivering higher data rates, improved spectral efficiency, and extended transmission distances. To meet these ever-growing and ambitious demands of modern connectivity, researchers are delving into pioneering solutions. This includes leveraging artificial intelligence algorithms, developing novel materials, exploring the potential of quantum communication, and advancing fiber optic networks. In this dynamic landscape, the integration of $PtSe_2$/ultrathin Al_2O_3/Ge- based photodetectors (PD) into optical frameworks stands out as a pivotal development. The successful integration of these three components - Platinum diselenide ($PtSe_2$) is deposited onto a thin layer of Aluminum Oxide (Al_2O_3) known as sapphire, which is itself placed on a Germanium (Ge) substrate - into photodetector, has emerged as a frontrunner, heralding a new era of efficiency and performance in data transmission. Their exceptional promise lies in their strong absorption in the Near-Infrared (NIR) range makes these photodetectors suitable for NG optical communication systems like long-distance data transmission in optical fiber and Free Space Optic (FSO) networks. It is demonstrated that under 1550 nm illumination, the $PtSe_2$/ultrathin Al_2O_3/Ge PD exhibits outstanding performance, achieving a responsivity of 4.24 A/W, a high specific detectivity of 4.47×10^9 Jones (excellent sensitivity), a rise/fall time (response speed) of $94.4/67.1\ \mu s$, and a light-to-dark current ratio of 1.15×10^5 (indicates minimal dark current and efficient light detection), even without applied voltage. Furthermore, applying a reverse bias of $-5\ V$ significantly enhances the responsivity to 16.32 A/W, further demonstrating the photodetector's ability to convert light into electrical current more efficiently. The response speed also benefits from the applied voltage, reaching $29.8/14.1\ \mu s$, indicating a faster response to changes in light intensity. Miniaturization offers additional benefits in terms of faster response times (rise/fall time of $32.6/18.9\ \mu s$ under zero bias and $9.6/7.7\ \mu s$ when applying a $-5\ V$ bias) and increased responsivity (38.18 A/W), making it potentially suitable for applications requiring high-speed light detection.

This research investigates the potential of $PtSe_2$/ultrathin Al_2O_3/Ge PDs to revolutionize NG optical communication systems compared to conventional detectors. The focus lies on designing a $1550\,nm$ FSO system using OptiSystem software. By leveraging advanced modeling tools, the integration of this photodetector within the FSO system is comprehensively evaluated, paving the way for a performance analysis of its impact on the overall communication system. Our results demonstrate that $PtSe_2$/ultrathin Al_2O_3/Ge - based PD exhibits superior performance metrics compared to conventional PDs, including a remarkable Q-Factor and a low Bit Error Rate (BER). Under a clear climate, the highest Q-factor of 9.84 and lowest BER of $3.44e-23$ are achieved, indicating optimal signal quality and enabling the system to operate at its longest achievable range. Light rain introduces a moderate decline, with a Q-factor of 6.75 and BER of $6.93e-12$, while light fog shows a Q-factor of 7.38 and a BER of $7.48e-14$.This translates to an even shorter operational range compared to both clear climate and light rain.These observations demonstrate the sensitivity of FSO systems to varying weather conditions. These outcomes underscore the system's outstanding robustness and reliable data transmission capabilities In conclusion, our study highlights the potential of $PtSe_2$/ultrathin Al_2O_3/Ge -based photodetectors as a promising avenue for enhancing the performance and functionality of NG optical systems, paving the way for advancements in telecommunications.

Keywords: Next Generation (NG), Free-Space Optical (FSO), $PtSe_2$/ultrathin Al_2O_3/Ge, Q-Factor, Bit Error Rate (BER)

Corresponding Email: rima.kebaili@univ-sba.dz

References

[1] Al-Gailani, S. A., Salleh, M. F. M., Salem, A. A., Shaddad, R. Q., Sheikh, U. U., Algeelani, N. A., & Almohamad, T. A. (2020). A survey of free space optics (FSO) communication systems, links, and networks. *IEEE Access*, *9*, 7353-7373. 10.1109/ACCESS.2020.3048049

[2] Samy, R., Yang, H. C., Rakia, T., & Alouini, M. S. (2023). Hybrid SAG-FSO/SH-FSO/RF transmission for next-generation satellite communication systems. *IEEE Transactions on Vehicular Technology*, *72*(11), 14255 – 14267. 10.1109/TVT.2023.3281256

[3] Abd El-Mottaleb, S. A., Singh, M., Alshathri, S., El-Shafai, W., & H. Aly, M. (2023). Enhancing security and capacity in FSO transmission for next-generation networks using OFDM/OCDMA-based ICSM codes. *Frontiers in Physics*, *11*, 1-12. 10.3389/fphy.2023.1231025

[4] Cao, F., Liu, L., & Li, L. (2023). Short-wave infrared photodetector. *Materials Today*, *62*, 327-349. https://doi.org/10.1016/j.mattod.2022.11.003

[5] Gundepudi, K., Neelamraju, P. M., Sangaraju, S., Dalapati, G. K., Ball, W. B., Ghosh, S., & Chakrabortty, S. (2023). A review on the role of nanotechnology in the development of near-infrared photodetectors: materials, performance metrics, and potential applications. *Journal of Materials Science*, *58*(35), 13889-13924. https://doi.org/10.1007/s10853-023-08876-8

[6] Dong, T., Simões, J., & Yang, Z. (2020). Flexible photodetector based on 2D materials: processing, architectures, and applications. *Advanced Materials Interfaces*, *7*(4), 1-18. https://doi.org/10.1002/admi.201901657

[7] Khosravian, E., Mashayekhi, H. R., & Farmani, A. (2021). Highly polarization-sensitive, broadband, low dark current, high responsivity graphene-based photodetector utilizing a metal nano-grating at telecommunication wavelengths. *JOSA B*, *38*(4), 1192-1199. https://opg.optica.org/josab/abstract.cfm?uri=josab-38-4-1192

[8] Zhu, Q., Chen, Y., Zhu, X., Sun, Y., Cheng, Z., Xu, J., & Xu, M. (2023). High-performance near-infrared PtSe2/n-Ge heterojunction photodetector with ultrathin Al_2O_3

O-36

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Title: The Effect of the Electrodes Interface on Dye-Sensitised Solar Cell (DSSC) Performances

Atouani Toufik[ab], *M. Boukais* [cd], *B. Dennai* [ab]

[a]*Matter Sciences Department, Faculty of Exact Sciences, University Tahri Mohammed Béchar Algeria.*
[b]*Laboratory for the Development of Renewable Energies and their Applications in Saharan areas (LDREASA)*
[c]*Higher School in Electrical and Energy Engineering of Oran, Algeria*
[d]*Research Unit of Materials and Renewable Energies (URMER), University AbouBakrBelkaïd, B.P. 119, Tlemcen, Algeria*

Abstract:

This paper presents a precise method for measuring tension losses at the interface of dye-sensitized solar cells (DSSC). The Schottky barrier model, which is based on the thermionic emission theory and the Nernst expression, is used to describe electron transfer at TCO/TiO2 and electrolyte/counter-electrode. This latter is used to calculate the concentration of a redox mediator couple in the electrolyte near the counter-electrode.
Tension losses at the DSSC's two interfaces were found to be considerable when the Schottky barrier height and active layer porosity surpassed the critical thresholds. These losses have an impact on the maximum power point (MPP), but not the short-circuit current (Jsc) or open-circuit tension (Voc).

Key words: *Solar cell; the tension losses; interface; DSSCefficiency*

Corresponding Email: atouani.toufik@univ-bechar.dz

References

[1] M. Grätzel,"Mesoscopic Solar Cells for Electricity and Hydrogen Production from Sunlight," Chem. Lett., vol. 34, no. 1, pp. 8–13, 2005.
[2] Ball, J. M., Lee, M. M., Hey, A., & Snaith, H. J, " Low-temperature processed mesosuperstructured to thin-film perovskite solar cells," Energy & Environmental Science,

O-37

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Optimization of Sn_2S_3 BSF layer to imporove CIGS thin film solar cells

Wafà BENSTAALI[a,b],

[a]Science and Techniques department, Faculty of Sciences and Technology, Abdelhamid Ibn Badis University,B. P. 227, Route deBelhacel, 27000 Mostaganem, Algeria.
[b]LPPMCA Laboratory of Plasma Physics, Conductive Materials and Their Applications, University of Science and Technology of Oran Mohamed Boudiaf, 31000 Oran, Algeria

Abstract:

Copper–indium–gallium–diselenide Cu(In,Ga)Se_2 (CIGS) is a semiconductor compound with a chalcopyrite crystal structure, that is promising for the development of high-performance photovoltaic applications. This is due to its high absorption coefficient, law cost and conversion efficiency. However, CIGS solar cells are limited by the toxic materials used in their layers as indium (In) and gallium (Ga) [1]. To improve devices performance, intensive efforts have been reported for the promotion of the quality of CIGS solar cells, one way is to introduce a back surface field (BSF) between the absorber and molybden layers. A variety of materials have been used to improve solar cell performance, such as MoS_2[2], V_20_5[3], and SnS[4]. On the other hand, rearchs have recently focused on the low-cost and eco-friendly Sn2S3 materials which have high stability. Sn_2S_3 includes Sn (Tin) and S (Sulfer) which are both abundant on earth[5]

In the present work, a ZnO/CdS/CIGS/Sn_2S_3 structure for thin film solar cells is numerically analyzed, using the one-dimensional SCAPS-1D simulator [6]. In order to obtain the optimal absorber layer thickness, we evaluate the influence of the BSF (thikness and doping concentration) on the electrical parameters of CIGS solar, such as open circuit voltage (V_{OC}), short circuit current density (J_{SC}), fill factor (FF), and power conversion efficiency (PCE). The results show that, after optimization of BSF and Absorber layers, a maximum conversion efficiency of about 26% was achieved with a 0.9 µm CIGS absorber layer and a thik Sn_2S_3 BSF layer

Key words: Ultra-thin CIGS; Sn_2S_3 , BSF layer; Conversion Efficiency

Corresponding Email: wafabenstaali7@yahoo.fr

ICMSE'2024

The 3rd Edition of the International Conference on Materials Science and Engineering and Their Impact on the Environment

Title: Modeling for Electrical Conductivity of Polymer/Graphene Nanocomposites

Maroua Nihel BENABDALLAH[a], Hayat BENAHMED[a], Sidi Mohamed BENHAMOU[b]

[a]Maroua Nihel BENABDALLAH, Hayat BENAHMED' Macromolecular Research Laboratory (LRM), Department of Physics, Faculty of Sciences, Abou Bekr Belkaid University, BP 119, 13000 Tlemcen, Algeria
[b]Sidi Mohamed BENHAMOU' Department of Secondary Cycle, Electrotechnical Branch, Higher School of Applied Sciences of Tlemcen, BP 165 RP Bel Horizon, 13000 Tlemcen, Algeria

Abstract:

In order to deepen the fundamental knowledge between the electrical conductivity of graphene/polymer nanocomposites in the case of a two-dimensional (2D) distribution of graphene nanosheets and their physic-chemical properties, this work is devoted to a theoretical approach to the electrical properties of such polymeric system. This study based on Mark Weber and Musa R. Kamal's theoretical model developed by Yasser Zare et al., which is developed to accommodate a two-dimensional (2D) distribution of graphene nanosheets. To this end, we have investigated the effects of graphene dimensions, its volume fraction in conductive networks, contact diameter, number of contacts between graphene nanosheets, orientation angle, interphase thickness and of the tunnel distance on the electrical conductivity of nanocomposites. The main conclusion is that the studied parameters affect drastically the electrical properties of the system under consideration.

Keywords: Conductivity electrical, graphene nanosheets, polymer/graphene nanocomposite, two-dimensional (2D) random distribution.

Corresponding Email: marouanihel45@gmail.com

O-39

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Elaboration of polymer network hydrogel for the removal of dyes from wastewater

Manel Safia CHOUIKHI[a], Salah HAMRI[a,b], Zakia HADJOU BELAID[a], Fayçal DERGAL[b], Djahida LERARI [b]

[a] Macromolecular Research Laboratory (LRM), Department of Physics, Faculty of Sciences, University of Abou Bekr Belkaid, PB 119,13000 Tlemcen, Algeria
[b] Center for Scientific and Technical Research in Physico-chemical Analyzes (CRAPC), PB384, Bou-Ismail, RP Tipasa 42004, Algeria

Abstract: Water is the liquid of life; it is necessary for human consumption, sanitation, and agriculture. This liquid's contamination causes numerous ailments and makes life tough. A substance called dye renders water useless and poses a serious risk to people, pets, and vegetation. Regrettably, the textile sector pollutes this priceless liquid by discharging wastewater into rivers, seas, and other water sources.

A clever substance that can draw color from an aqueous medium is known as a hydrogel, a polymer network having the capacity to absorb water as well as other molecules such as organic pollutants like dyes. Their hydrophilic nature makes it possible to eliminate pollutants by interacting with the water present in their structure.

The goal of this work is an elaboration of a superabsorbent hydrogel with excellent properties such as hydrophilicity and high swelling capacity that can absorb and retain considerable amounts of dye molecules in an aqueous solution.

Key words: Hydrogels, polymer network, superabsorbent, wastewater, adsorption, dyes.

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Optimizing thermal management and temperature control of building brick walls through integration of phase change materials: A case study in Bechar city.

Bachir ALLAM, Taieb NEHARI, Mohamed HADJADJ, Assala ZEHOUANI

Smart Structures Laboratory (SSL), University of Ain Témouchent-Belhadj Bouchaib, Ain Témouchent, Algeria

Abstract:

One of the largest consumers of energy is the building sector, where nearly 30% of total energy is consumed by space cooling. The foundation for achieving zero-energy buildings is the utilization of renewable energy sources and energy conservation within the building envelope to enhance thermal comfort and reduce energy consumption. For this propos this paper presents a numerical study on the heat transfer characteristics of a porous brick filled with phase change materials (PCMs) in typical days of July 2021 in Bechar city (Algeria). Within the thermal model presented in this study, the PCM is filled into the square cavities of the bricks. The 2D numerical simulation was conducted utilizing Ansys Fluent software, employing finite volume analysis and the enthalpy porosity-based approach. The effectiveness of the integration of PCM in the building bricks has been evaluated by comparing two different cases - the normal bricks and bricks with PCM filled in the square cavities. Furthermore, the study was conducted with four different PCMs. The findings revealed that using PCM in building bricks stabilizes and reduces indoor temperature fluctuation. Using Capric acid as a PCM shows the lowest maximum temperature of 27.8°C with the peak indoor heat flux decreased by 34% and shifted by 2.5h.

Key words: Solar energy storage; Energy consumption; Building brick; Phase Change Materials; Thermal comfort

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

The impact of material choices on greenhouse gas emissions and climate change

mekhloufi belkacem

Abstract

The impact of material choices on greenhouse gas emissions and climate change underscores the critical role that our decisions regarding materials play in shaping environmental outcomes. This impact is multifaceted, encompassing various stages of the material lifecycle, from extraction and processing to transportation, use, and disposal. Key factors influencing this impact include the carbon intensity of materials, energy requirements for their production, and emissions associated with extraction and manufacturing processes. For instance, materials like cement and steel are particularly carbon-intensive due to the energy-intensive processes involved in their production, leading to significant greenhouse gas emissions. Furthermore, the use of certain materials can exacerbate deforestation, habitat destruction, and other environmental degradation, indirectly contributing to climate change. For example, the extraction of timber for construction or paper production can lead to loss of carbon sinks and biodiversity. Addressing this issue requires a holistic approach that considers not only the direct emissions associated with materials but also their broader environmental and social impacts. Strategies for mitigating the impact of material choices on climate change include adopting sustainable material alternatives, optimizing production processes to reduce energy

consumption and emissions, promoting recycling and circular economy practices, and implementing policies and regulations that incentivize environmentally responsible choices. By prioritizing the use of low-carbon, renewable, and recyclable materials and embracing innovative technologies and design strategies, we can minimize the environmental footprint of materials and contribute to global efforts to combat climate change and promote sustainability.

.

O-42

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Title: Investigations of physical aspects of spinel AAl_2O_4 oxides via ab-initio calculations

BLAHA Lamia Farah[a], KHATIR Radja[b], AMERI Ibrahim[c], …

[a]Laboratory of Physical Chemistry of Advanced Materials (LPCMA), University of Djillali Liabes, Sidi-Bel-Abbes, Algeria.
[b]Laboratory of Electrical Engineering and Materials (LGEM), The Higher School of Electrical and Energetic Engineering (ESGEE), Oran, Algeria.
[c]Laboratory of Physical Chemistry of Advanced Materials (LPCMA), University of Djillali Liabes, Sidi-Bel-Abbes, Algeria

Abstract:

Text of the abstract

The physical properties of AAl_2O_4 have been studied in this article using semi-classical Boltzmann transport theory and the full-potential linearized augmented-plane-wave approach throughout Density functional theory. The BoltzTraP code is used to calculate the thermoelectric properties, whereas the WIEN2k code is utilized to calculate the electronic and magnetic characteristics. Density of states (DOS) and spinpolarized band structures (BS) calculations revealed that the materials under study are half-metallic by nature. The FM state was identified as the stable ground state for these materials through an analysis of the energy stability of the ferromagnetic (FM) and antiferromagnetic (AFM) states. Exchange energies, hybridization, and John-Teller energy confirm that electron spin, is the source of ferromagnetism in these compounds. In addition, we thoroughly examined these compounds' spin polarization and Curie temperature. The ratio of electrical to thermal conductivity fits the Wiedmann Franz law, according to thermoelectric property investigations. The investigated compounds' adequate thermoelectric efficiency was shown by the thermoelectric power factors and figures-of-merit.

O-43

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Structural, Electronic, Optical, and Thermodynamic Properties of Copper Halide CuCl1-xIx (0.0 <= x <= 1.0) Ternary Alloy: First Principal Calculations

AMERI Mohammed[a], BLAHA Lamia Farah[a], KHATIR Radja[b]

[a]University Djillali Liabbes Sidi Bel Abbes . Physico-Chemiistry Laboratory of Advanced Materials
[b] Laboratory of Electrical Engineering and Materials (LGEM), Oran, 31000, Algeria

Abstract

First-principles calculations of the physical properties of ternary CuCl1-xIx alloys using the Full Potential Linearized Augmented Plane Wave (FP-LAPW) method based on density functional theory (DFT) within the local density approximation (LDA), are presented. The equilibrium lattice constants and volume modulus are compared to other experimental and theoretical results using the GGA generalized gradient approximation. The concentration dependence of the electronic band structure and the direct-indirect bandgap structures are also studied. Furthermore, the thermodynamic stability of CuCl1-xIx ternary alloys is studied by calculating the excess enthalpy of mixing ΔHm as well as the phase diagram.

.

O-44

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Title: Electrochemical characterization of the AMX anion exchange membrane in buffered solution.

Abdallah Timmaoui[a], Mahmoud Ferhat[a]

[a] Matter sciences Department, Faculty of sciences, University of Laghouat, Algeria.

Abstract:

Membrane technology has gained increasing significance in industrial separation processes, desalination, and wastewater treatment. It plays pivotal roles in various industries such as food processing, pharmaceuticals, and petrochemicals. Over the past two decades, membrane technology has been increasingly utilized to tackle water scarcity through wastewater reclamation and desalination. Electrodialysis (ED) stands out as one of the most prevalent membrane separation processes, driven by an electric field gradient enabling the separation of minerals from feedwater solutions. It generates two distinct streams - a desalinated flow termed diluate and a concentrated flow termed concentrate. However, operational challenges in electrodialysis may arise, including inorganic salt precipitation on membrane surfaces, membrane degradation, and elevated energy consumption due to concentration polarization at the membrane-solution interface during mass transport. A comprehensive understanding of concentration polarization is crucial for enhancing membrane performance, process efficiency, and reducing operational costs. In this study, we enhanced mass transport through the membrane by introducing an ammonia buffer. Results demonstrate that ammonia addition facilitates counter-ion transfer, completely eliminating system polarization, and catalytically enhancing the water dissociation reaction in the boundary layer. This shift towards ohmic regions by destruction and elimination of the diffusion boundary layer improves overall process efficiency.

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Effect of Annealing and Plasticization on the Crystallization and Thermo-mechanical Properties of Poly(lactic acid)

Lina benkraled[a], Latifa Zair[a], Khadidja Arabeche[a], Assia Zennaki[a], Abdelkader Berrayah[a],

[a]Department of Physics, Laboratoire de Recherche sur les Macromolécules (LRM), University of Tlemcen, Algeria

Abstract:

Recently, there has been an increasing interest in biopolymers to substitute petroleum-based plastics in many applications. Among commercially available biopolymers, poly(lactic acid) (PLA) is the most promising. It is a biodegradable and compostable thermoplastic, derived from 100 % renewable feedstocks. Besides being environmentally friendly material, PLA offers good mechanical properties, high transparency and easy processability. However, the large-scale industrial use of PLA is restricted mainly by its inherent brittleness, poor thermal resistance and slow crystallization kinetics. Various strategies have been investigated to overcome these shortcomings such as incorporation of fillers and blending with other polymers. This work aims to improve the properties of PLA by thermal annealing and plasticizer addition. PLA was plasticized with low molecular weight poly polyethylene glycol (PEG-400) at a content of 10 wt% using solvent casting method. The plasticized and non-plasticized films were annealed at different temperatures (80-120 °C) then analyzed with differential scanning calorimetry (DSC) and dynamic mechanical analysis (DMA). The results showed an improvement of the crystallinity and heat resistance with annealing for all samples. The crystallinity increased with increasing annealing temperature for both plasticized and non-plasticized samples, but the plasticized materials showed higher crystallinity. The PEG addition also altered the content of the α′ and α crystalline forms.

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Synthesis and Characterization of Polymer-Based Nanocomposites Reinforced with Magnesium-Aluminum and Zinc-Aluminum Layered Double Hydroxides.

HAFFAF Wissem[a], M. Hamouni [a], Z. Abdelsadak.[b].

[a] University Abubekr Belkaid, Faculty of Science, Macromolecules Research Laboratory (MRL),Tlemcen, Algeria.
[b] Institute of Electrical and Electronics Engineering, University of M'hamed-Bougara, Independence Avenue, 35000, Boumerdès, Algeria.

Abstract

Layered double hydroxides (LDHs) are a type of anionic clay that have been studied for their potential in creating polymer nanocomposites with enhanced mechanical properties, thermal stability, and flame retardancy. Consequently, these materials have found wide-ranging applications across various fields and industrial sectors [1-2].

The aim of this work is to examine the role of divalent metal cations on the thermal and the mechanical properties of nanocomposites. Two different LDH materials were synthesized using aluminum (Al^{3+}) as a trivalent cation (M^{3+}) with varying M^{2+} cations such as magnesium (Mg^{2+}) and zinc (Zn^{2+}) ions to prepare magnesium–aluminium-layered double hydroxide (MgAl-LDH) and zinc–aluminium-layered double hydroxide (ZnAl-LDH). The samples were prepared by the co-precipitation method with a molair ratio M^{2+}/M^{3+}=3. These nanocomposites were prepared by dispersing the nanofillers into a polystyrene matrix via the solvent mixing technique. The effects of these two types of LDHs on dispersion, thermal, and mechanical properties of nanocomposites were studied using various technical analyses: Fourier transform infrared spectroscopy (FTIR), X-ray diffraction (XRD), dynamic mechanical analysis (DMA) and differential scanning calorimetry (DSC).

According to the results obtained from XRD indicated that intercalated/exfoliated structure were achieved in the polystyrene matrix. DMA and DSC analysis suggested that the storage modulus and T_g for the PS/LDHs nanocomposites was efficiently improved.

Key words:
Polystyrene, Layered double hydroxides (LDHs), Nanocomposites, ZnAl-LDH, MgAl-LDH.

Corresponding Email: wissemhaffafdz@gmail.com

References

[1] KUMAR, Manish, CHAUDHARY, Vivek, SURESH, Kelothu, et al. Synthesis and characterization of exfoliated PMMA/Co–Al LDH nanocomposites via solvent blending technique. Rsc Advances, 2015, vol. 5, no 50, p. 39810-39820.

[2] BARIK, Sunita, BADAMALI, Sushanta Kumar, BEHERA, Lingaraj, et al. Mg–Al LDH reinforced PMMA nanocomposites: A potential material for packaging industry. Composite Interfaces, 2018, vol. 25, no 4, p. 369-380.

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Investigation des propriétés structurales des nitrures de métaux de transition

TAYEBI Nadjia[1] , BLAHA Lamia Farah[1] and KHATIR Radjaa[2]

[1]Laboratoire Physico-chimie des Matériaux Avancés (LPCMA), Université Djillali Liabès, Sidi Bel- Abbès 22000, Alegria.
[2]Laboratory of Electrical Engineering and Materials (LGEM), The Higher School of Electrical and Energetic
Engineering (ESGEE), Oran, Algeria.

Abstract:

Les progrès technologiques et industriels dépendent fortement de l'état d'avancement des matériaux. Le développement des simulations informatiques a favorisé des études importantes dans le domaine de la matière condensée. Depuis plus de deux décennies, Les composés à base de métaux de transition présentent un grand intérêt pour les scientifiques.

Dans ce travail, les propriétés structurales des nitrures de métaux de transition **XN (X = Cr, V, Co, Mn)** ont été étudiées dans les deux phases cristallines : la phase Zinc Blende et la phase rocksalt NaCl avec la méthode **(FP-LMTO)** [1-2] qui se base sur la théorie de la fonctionnelle de la densité **(DFT)** [3]. L'approximation de la densité locale **(LDA)** et l'approximation de la densité à spin local **(LSDA)** ont été utilisées**.** Le paramètre de réseau, le module compressibilité et sa dérivé ont été calculés Les résultats obtenus ont été comparés avec les résultats théoriques et expérimentaux disponibles et ils sont compatibles entre eux.

Il est clair que la structure du composé VN de type RS est plus stable par rapport à ZB. Alors que les composés CrN, MnN et CoN sont plus stables dans la structure zinc-blende.
Nos résultats sont en bon accord avec d'autres valeurs théoriques trouvés dans la littérature. Les calculs du module de compressibilité des nitrures de métaux de transition CrN, VN, CoN et MnN indiquent que la phase RS est plus dure par rapport à la phase ZB.

Key words: nitrures de métaux de transition, méthode (FP-LMTO), DFT, LDA et LSDA, stabilité structurale.

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

The 3rd edition of the international conference on matériels science and engineering and their impact on the environment

The Determinants of PermeableConcreteBehavior:ExploringIntrinsicCharacteristics

Chaabane Lynda Amel [a], Ouhib Rachid [a], Bouyakoub Amel Zahira [a], Harrache Djamila[a], Boudelel Bochera[b], Medelci Djezzar Khadidja[b]

[a]Laboratoire Physico Chimie Es Materiaux Avances, Sidi Bel Abbes, Algeria.
[b]Student in Materials, Department of Civil Engineering and Public Works Faculty of Technology, DjillaliLiabes University, B P 89 SidiBel Abbes, Algeria.

Abstract:

Le béton drainant (également connu sous les noms de béton poreux ou perméable) est spécialement formulé pour présenter une porosité élevée, favorisant ainsi l'absorption et le drainage de l'eau. Il est couramment utilisé dans la construction de dallages et de chaussées. L'utilisation du béton drainant a considérablement augmenté à travers le monde en raison de ses propriétés de drainage. Ses applications les plus fréquentes incluent les aires de stationnement, les routes piétonnes et carrossables, les piscines, les aires de jeux et les terrains de tennis.

Le béton perméable (également appelé béton poreux ou perméable) est spécialement formulé pour avoir une porosité élevée, favorisant ainsi l'absorption et le drainage de l'eau. Il est couramment utilisé dans la construction de pavés et de trottoirs. L'utilisation du béton perméable a considérablement augmenté à travers le monde en raison de ses propriétés drainantes. Ses applications les plus courantes comprennent les aires de stationnement, les routes piétonnes et carrossables, les piscines, les terrains de jeux et les courts de tennis.

Dans cette étude, nous nous concentrons spécifiquement sur le béton drainant, également appelé béton perméable ou caverneux. Nous avons entrepris la fabrication et l'analyse d'un

béton drainant, en commençant par une caractérisation approfondie des matériaux utilisés, suivie par l'étude du processus de fabrication du béton en question. Par la suite, des essais mécaniques ont été menés à différents stades de durcissement du béton.

Dans cette étude, nous nous intéressons spécifiquement aux bétons perméables, également appelés bétons perméables ou caverneux. Nous avons entrepris la fabrication et l'analyse d'un béton perméable, en commençant par une caractérisation approfondie des matériaux utilisés, suivie de l'étude du procédé de fabrication du béton en question. Par la suite, des essais mécaniques ont été réalisés à différentes étapes de durcissement du béton.

Les résultats de ces tests ont montré une prise initiale du béton après environ 4 heures, avec une solidification significative atteinte après 24 heures. Cette rapide prise initiale est essentielle pour assurer la résistance précoce du béton et sa capacité à supporter des charges légères.

Les résultats de ces essais ont montré une prise initiale du béton au bout de 4 heures environ, avec une solidification significative obtenue au bout de 24 heures. Cette prise initiale rapide est essentielle pour assurer la résistance précoce du béton et sa capacité à supporter des charges légères.

Key words: béton drainant- formulation- caractéristiques intrinsèques.Mots clés : béton perméable- formulation- caractéristiques intrinsèques

Corresponding Email: chaabane25@hotmail.com

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

The 3rd edition of the international conference on matériels science and engineering and their impact on the environment

Industrial Textile Wastewater Treatment And Potential Of Reuse

Rachid Ouhib[a], Djahaf Kaouthar[a], Chaabane Lynda Amel[a], Amel Zahira Bouyakoub[a] , Harrache Djamila[a], Belhadj Hafida[a]

[a]laboratoire Physico Chimie Es Materiaux Avances, Sidi Bel Abbes, Algeria

Abstract :

In this study, a textile effluent which is the primary cause of water pollution was treated by a combined process, with a view to possible reuse. The optimal electroflottation conditions were determined under optimal conditions for maximum dye removal. The results show that the effluent treated by this combined method contained essentially no turbidity, color or COD. The treated effluent quality satisfied the requirement of water. Therefore, textile wastewater reclamationand reuse is a promising alternative, which can both conserve the available water resource and reduce or eliminate the environmental pollution.

Keywords: textile waste water, Pollution, impact, Water reuse.

Corresponding Email : r_ouhib@yahoo.fr

O-50

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Ab initio full-potential study of properties and magnetic phase stability of rare earth diboride compounds

F.Zazoua[a], A.Z. Bouyakoub[b], R.Ouhib[c]

[a]Djilali Liabès University of Sidi Bel Abbès , Algeria

Abstract:

We study the structure and magnetic phase stability of rare earth diboride compounds, RB_2, using density functional simulation within the local density approximation. At zero pressure the hexagonal (P6/mmm) structure is energetically stable and at high pressure these materials prefer to keep the same structure. Bulk modulus, shear modulus of all the hexagonal compounds have been calculated[1] [2] . The pressure dependance of the volume is determined. The structural parameters and magnetic phase stability for RB_2 (R= Tb, Dy, Ho,Er, Tm, and Yb)compare quite well will experimental results. For the others rare earth materials, our results are prediction.

Key words: rare earth, compounds, Electronic structure.

Corresponding Email:

References

[1] J. P. Perdew and Y. Wang, Phys. Rev. B 45, 13244 (1992).

[2] V. I. Anisimov, J. Zaanen, and O. K. Andersen, Phys. Rev. B 44, 943 (1991).

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Lignin-Phenylhydrazone as a Corrosion Inhibitor of API X52 Carbon Steel in 3.5%NaCl and 0.1 mol/L HCl Medium

Nabila AISSIOU[1,2], Moussa BOUNOUGHAZ[2] and Amel DJEDDI[2].

1. Polymeric Materials Laboratory, Faculty of Chemistry, University of Science and Technology Houari Boumediene, BabEzzouar, 16111 Algiers, Algeria.
2. Laboratory of Polymers Treatmentand Forming, Faculty of technology, MHamed Bougara University, 35000, Boumerdes, Algeria

Abstract:

The best alternative to fight against corrosion is the use of aninhibitor, the purpose of this work is the formulation of a newbiomass-based molecule against corrosion of carbon steel. Lignin was extracted using the Kraft process and phenylhydrazine molecules have been scratched. The influence of the lignin-phenylhydrazone(LP) on the corrosion of carbon steel in salt and the acidic medium was studied by the polarization resistance, the potentiodynamic polarization, and the electrochemical impedance spectroscopy. The results of these tests reveal that the behavior of the inhibitor is a mixed type. The adsorption mechanism of the inhibitor follows the Langmuir isothermal model. Gibbs energy shows that the process of inhibition of carbon steel is spontaneous. The SEM confirms that the inhibitor reduces the corrosion of the steel and stops the corrosion pitting phenomenon. The modified lignin shown as a good corrosion inhibitor in acid medium is highly saline with an efficiency> 96%.

Key words: Kraft Lignin; Phenylhydrazone; Corrosion inhibitor; Corrosion pitting;

O-52

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Title: First-principles investigation of: AgBr1−xIx (0 ≤ x ≤ 1) ternary alloys

KHATIR Radja[a,b], BLAHA Lamia Farah[c], AMERI Ibrahim[c], KESSAIRI Khadra[a]

[a]Laboratory of Electrical Engineering and Materials (LGEM), The Higher School of Electrical and Energetic Engineering (ESGEE), Oran, Algeria.
[b]Materials and Sustainable Development Department (LMCDD), Faculty of Science, University of Sidi-Bel-Abbes, Sidi-Bel-Abbes, 22000, Algeria
[c]Laboratory of Physical Chemistry of Advanced Materials (LPCMA), University of Djillali Liabes, Sidi-Bel-Abbes, Algeria

Abstract:

We report structural, electronic, and optical properties of AgBr1−xIx ternary semiconductor alloys investigated in the rocksalt (B1) and zinc blend (B3) structures using the full-potential linearized augmented plane-wave (FP-LAPW) method based on the density functional theory implemented in the WIEN2k code. For treating the exchange–correlation potential term, we have chosen the generalized gradient approximation (GGA) and the total energy approach is used to determine the equilibrium volume. The lattice constants, for the B1 and B3 phases, versus iodide concentration (x) were found to deviate slightly from the linear relationship of Vegard's law. The energy gap is found to be direct in B3 phase for our alloys. In addition to that, a detailed description of the electronic properties such as band structures and density of states has been also performed. To our knowledge, there are no correlative experimental and calculated results about the dielectric function for this alloy so we consider the present results as a prediction study

Key words: DFT, FP-LAPW, GGA, Electronic structure, Optical properties.

Corresponding Email:
Khatir_rajaa@hotmail.fr

O-53

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Étude des propriétés structurales et électronique des matériaux piézoélectrique: premier principe de l'effet de la pression.

Rachedi.S[a], Moulay.N[b], Benamara. A[b]

[a]*Microscopy,MicroanalysisofMatterandMolecularSpectroscopyLaboratory,UniversityofDjillaliLiabesofSidi BelAbbes,Algeria*
[b]*Physical-ChemistryofMaterialsLaboratory, UniversityofAMMAR TilidjiLaghouat,Algeria*

Résumé

Dans cet article, nous avons analysé les caractéristiques structurelles. Les propriétés électroniques, élastiques des deux structures cristallines cubiques de type pérovskite sont présentes dans le BiAlO3 et le BiScO3 en utilisant la méthode des ondes plates linéaires augmentées avec un potentiel total (FPLAPW). Cette méthode est basée sur la théorie de la fonction de densité. (DFT). Pour décrire avec précision le potentiel d'échange et de corrélation, nous avons utilisé l'approximation de gradient généralisé (GGA) et son correspondant GGA-PBE. Les caractéristiques des états réels qui ont été calculés sont, dans une large mesure, en accord avec les données d'observation. Dans cet article, nous avons examiné plusieurs types différents de pérovskite, et deux d'entre eux, BiMO3 (M = Al, Sc), étaient de la pérovskite de bande indirecte. En outre, la stabilité mécanique des deux composés a été prouvée par leurs caractéristiques élastiques. Nous avons étudié diverses propriétés électroniques pour déduire les caractéristiques des deux matériaux piézoélectriques.

Mots clés : pérovskites, premier principe, propriétés piézoélectriques, GGa,

Corresponding Email: rachdisamia@yahoo.fr

References:

[1] C.KittelIntroductiontoSolidStatePhysics6thedn(NewYork:Wiley)(1986).
[2] J.F.Nye,PhysicalpropertiesofCrystals,(OxfordUniversityPress),1985.

O-54

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Title: Enhanced photocatalytic activity of monometallic Ag, Cu nanoparticles loaded on ZnO prepared via modified polyol process

AbdElouahabNoua[*a], DoganKaya[a, b], FarukKaradag[a]and Ahmet Ekicibil[a]

[a] *Cukurova University, Department of Physics, Adana, 01330 Turkey*
[b] *Cukurova University, Department of Advance Materials and Nanotechnology, 01330 Turkey*

Abstract:

Zinc oxide is a well-known photocatalyst and different approaches were applied to enhance its photocatalytic performance, particularly under solar light irradiation[1, 2]. In this study, plasmonic materials were used to increase the absorption in the visible region in a form of a metal/ZnO system to improve charge carrier separation. Here, monometallic Ag and Cu nanoparticles were successfully reduced on ZnO using a modified polyol process. XRD, SEM, EDS, FTIR, and UV-Vis techniques were employed to investigate the NPs' different properties. The photocatalytic activity of the NPs was evaluated by the degradation of methylene blue dye in an aqueous solution under both direct sunlight irradiation and UV - light. The obtained results show that the metal/ZnO system exhibits good photocatalytic activity under UV light and even better efficiency under solar light with a degradation rate of 98% for Cu/ZnO NPs.

Key words: ZnO, bimetallic AgCu NPs, MB dye, Polyol process, Photocatalytic degradation.

Corresponding Email:anoua@cu.edu.tr

References

O-55

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Title: **Investigation of Structural and Magnetic Properties of Mn_2ZrP: A Heusler Compound with X_2YZ Formula**

Malika AMARI[1],Laboratory of Renewable Energy and Materials (LREM). University Yahia Fares of Medea, 26.000, Algeria

Abdelhamid CHELLALI[2], Laboratory of Biomaterials and Transport Phenomena (LBMPT), University Yahia Fares of Medea,Algeria.

Zakaria TRIKI[2,] Laboratory of Biomaterials and Transport Phenomena (LBMPT), University Yahia Fares of Medea,Algeria.

Faouzi DIDI[1],Laboratory of Renewable Energy and Materials (LREM). University Yahia Fares of Medea, 26.000, Algeria

Mustapha SAHNOUNE CHAOUCHE[1],Laboratory of Renewable Energy and Materials (LREM). University Yahia Fares of Medea, 26.000, Algeria

Fatma Zohra SAIDOUNE[2,] Laboratory of Biomaterials and Transport Phenomena (LBMPT), University Yahia Fares of Medea,Algeria

Abstract:

Mn2ZrP, a Heusler compound with the chemical formula X_2YZ, where Mn and Zr represent transition metals and P denotes a main group element, is investigated for its structural and magnetic properties. The crystal structure, magnetic ordering, and electronic structure of Mn_2ZrP are explored using experimental and theoretical techniques. The compound exhibits intriguing magnetic behavior, making it a potential candidate for applications in spintronics and magnetic data storage. This study provides insights into the fundamental properties of Mn_2ZrP, highlighting its significance in the field of materials science and condensed matter physics.

Keywords

Mn_2ZrP, Heusler compounds, crystal structure, magnetic properties, spintronics.

O-56

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Title: **Fine-tuning the strategy XtalOpt + Gibbs2 codes. Application to thermoelectric compounds (AgCl, PbTe and CoSb 3) under stress: Phase diagrams pT.**

H. CHORFI [a], H. MAOUDJ [a], A. BOULTIF [a], …

[a] Université des frere Mentouri, Constantine/Algeria

Abstract:

The ultimate objective of this work is the proposal of new materials with high thermoelectric performance. The success in its achievement is associated with the fulfillment of two other intermediate objectives. The first is of a methodological nature and consists on the combination of prediction models of crystalline structures with strategies for chemical-quantum calculation of electronic, thermodynamic and transport properties (VASP+newGIBBS). The second is of an applied nature. It seeks to obtain property-structure correlations from the computational exploration of regions of increasing pressures in the phase diagram of families of compounds with high value of the figure of merit (ZT) (AgCl, PbTe, SnSe, CoSb3) and allowing stoichiometric variations.

The code XtalOpt is a computational tool that makes use of evolutionary algorithms for the prediction of crystal structures based solely on the composition of a material system. The number of atoms in the unit cell that handles. XtalOpt can reach a hundred. It has been created entirely of Prof. Eva Zurek. Its set up to couple it with the code GIBBS2 supposes a novel computational strategy in the search for stable structures in specific regions of the phase diagram, created in the group TCCMAT at the University of Oviedo.

Key words: Thermoelectric materials, phase diagram, evolutionary algorithms,

Corresponding Email: h.chorfi@umc.edu.dz

O-57

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment.

Title: Magnetic, electronic, dielectric, optic , Properties of emergent inverse Heusler metamaterial: Rh_2HoSi .

Presenting author: Chafia Métaoui [a], Amal Dendane [b], Fatima Kerrouchi [c].

[a] - Department *of Physics , Faculty of Exact Science and Informatics*, *University- Hassiba Bouali of Chlef UHBC*, *Postal code : 02000 , Ouled Farès City, Country :* Algeria

LPCMA .Department *of Physics , Faculty -Exact Sciences , University of Djilali Liabes - Sidi Bel Abbesse SBA*, *Postal code : 22000* .Algeria.

LERM. Department *of Mechanic , Faculty of Sciences and Technology. University of Médéa. Postal code : 26000* . Algeria.

[b] Author 's Department *of Physics , Faculty of Exact Science and Informatics*, *University Bouali of Chlef UHBC*, *Postal code : 02000 , Ouled Farès City, Country :* Algeria .

[c] Author' s Department *of .Physics , Faculty of Exact Science and Informatics*, *University Bouali of Chlef UHBC*, *Postal code : 02000 , Ouled Farès City, Country :* Algeria

Extended Abstract:

A novel complex quantum multifunctional advanced meta material ,is predicted according to the first principle of *ab initio* material science method : (Rh_2HoSi) as Ternary Inverse Heusler : X_2YZ ,because atomic number (z) values are related such as : z(X) < z(Y) . Stoïchiometric composition is detailed like a mixture matter : 51.6041 % (Rh) ; 41.3539 % (Ho) ; 7.0420 % (Si) .Atomic Wyckoff components' s positions on molecular site geometry ,are indicated as follow : 4d(0,0 ,0) ⇢ (X_1) ; 4c (1/4 , 1/4, 1/4) ⇢(X_2) ; 4b (1/2 , 1/2, 1/2) ⇢ (Y) and 4a(3/4 , 3/4, 3/4) ⇢ (Z). Within : n = 4 atoms per molecule formula , as cubic FCC crystal ' structure .net work ,is like : z(Z) =14 < z(X) =45 < z(Y) = 67 , sample becomes of inverse type Hg_2CuTi ,it performs two (XY) (XZ), CFC sub-lattices, occupied and centered respectively by (X_1) and (X_2). Structural phase de Nowotny-Juza. : (XY) (XZ) is highly ordered crystallization : X_A , better stable than: L_{21} , with a space group : (Fm-3m), n°216 .Modeling system formalism based on DFT, considering Full Potential –Linear Muffin Tin Orbital Spheres (FP-LMTO) , adopting generalized gradient of electronic charges

density approximation (GGA) for exchanges and correlations ,stated by JP .Perdew and Y.Wang , in 1991 and 1996. We take in account : spin polarization SP (Up ,Dowm) .Firs step study is : investigating structural lattice parameters of stable equilibrium state point , using (GGA+ SP) method , taking in account Spin (S) Polarization (P),at absolute work conditions:[T_0 = 0 (K),P_0 =0 (GPa)]. Targeted crystal sample alloy is assumed to be a quantum well , undergoing stationary perturbation from external potential interaction , then complicated Schrodinger equation motion is solved for (N) bodies-particles .Physic-chemistry lattice parameters values, are deduced after applying Murnangham fit minimization - optimization for eigen molecular total energy (E) , are shown like below :

$a_{0\ moy}\ (\text{ua}) = 9.533879917$; $E_0\ (\text{Ry}) = -44978.2153$; $V_0\ (\text{ua})^3 = 433.29037$ . .

Artificial manufacturing possibility , is confirmed by crucial thermodynamic parameter with a negative Gibbs free energy : G [T= 0(K) , P =0 (GPa)] = - 0.20 (K J/mol). In precedent work study. Second step consists on investigating: magnetic, electronic, dielectric, optical, properties ,describing characteristic behaviors were finally obtained .When sample is submitted to a compressive different pressures ,at isothermal absolute temperature : T_0 = 0 (K) and variable P ={ 0 , 10 , 20 , 30, 40 ,50} (GPa),with resulting lattice parameter: a(P) , it occurs many influences on : total energy and all others characteristic behaviors . At isobaric absolute pressure : P_0 = 0(GPa) ,we check temperature effects influences from: T={ 0, 100 , 200 , 300 , 400 ,500,….→ 1600}(K).On predictive Slater –Pauling rule for magnetic behavior and half metallicity and total covalence electronic number : zt =29 , total magnetic moment may be related to three expressions next quoted : M= (Zt -24) =+ 5(μB) , then M = (Zt -28) =+ 1(μB) , but also M= (Zt -34) = - 5 (μB) , let's conclude the real statement coexistence of several original natural magnetism forms such as :(ferromagnetism , ferrimagnetisms , anti ferromagnetism) types are revealed Bands simulations , focused on stable equilibrium state point give values of partials intrinsic magnetic moments for each component, hence permit summing calculation for total molecular magnetic moment values : (M) ,varying versus increasing values about elementary irreducible Brilliouan zone cell's volume : (V). A deep exploration On possible eventual phases transitions, consists on changing variable work conditions [T (K), P(GPa)] so consequent on: lattice parameter , magnetic properties besides the influence of chemistry stoichiometry and atomic positions .with its appreciated considerable magnetism , sample (Rh2HoSi), exhibits a perfect metallic behavior as electronic conductor device , shown aspects are in : electronic Total DOS , electronic Fat bands , indicating Fermi Energy (E_F) presence in conduction band . Fermi energy variations according to (T,P) means : E_F (T) , E_F (P) , are all of them increasing shape , with increasing pressures. Variable pressures , at absolute temperature , display a certain range interval values for Fermi Energy : 26.1456 < E_F (ev) < 46.4519. For Spin (Down , Up) ,polarizations , at any conditions [T(K) , P(GPa)] ,sample alloy maintains metallic conductor behavior .Total dielectric permittivity function is a complex parameter , containing two parts : $\mathcal{E}_1$ (ω) is real part , $\mathcal{E}_2$ (ω) is imaginary part. Dielectric properties are interpreted with other parameters: Reflectivity: R(ω) vanishes at all for electromagnetic incident frequencies energy and Loss Electron Spectroscopy Energy : L (ω)lower than 0.1(ev) , giving low values , in favor for a good electric storage energy capacitance .Meta material aspect is announced , when the real dielectric permittivity function part is permanently negative. The imaginary part is positive , interpreting a good absorption inside targeted material with null reflectivity .The total optical refractive index function is a complex parameter with two parts : n - real is greater than 1.33 (water) , k-imaginary is

greater than 7 , in favor for a well beam radiation absorption and excitation phenomena scattering quasi particles. Frequency of optical conductivity function is probability: σ (ω) , with a good accordance to a usefully optical tool . The new meta material (Rh_2HoSi) is : magneto electronic, magneto optic ,will enhances surely : solar photovoltaic cells in (harvesting , storage , conversion , smart grids , transport , distribution , monitoring survey , security , repairing) , beam - matter interaction (probes , quantum boxes ,wires, detectors , screens) , optical density of medical imaging films , radars wave guide and telecommunication in military security defense , aerospace naviguations commandments boards , informatics memories, microprocessors .

Key words: Multifunctional Metamaterials; Heusler Alloys ; FP-LMTO ; DFT- GGA ; Spintronics ; Optophotoelectronics.

Corresponding Email: metaouichafia@gmail.com

Cellular Phone : (+213) 06 78 18 05 82 . / (+213) 05 54 09 69 47 .

References

[1] Tanja Graf, Claudia Felser, Stuart S.P.Parkin, Simple rules for the understanding of Heusler compounds, Progress in Solid State Chemistry.Volume 39, May 2011, Pages 1-50, science direct.
[2] A. De Freitas, P. Martín, E. Castro, J.L. Paz. Eigen values and eigen functions for the ground state of polynomial potentials. Physics Letters A, Volume 362, 2007. Pages 371-3374.
[3] Chaoyuan Zhu, Kuo Kan Liang, Michitoshi Hayashi, Sheng Hsien Lin. Theoretical treatment of anharmonic effect on molecular absorption, fluorescence spectra, and electron transfer.Chemical Physics, Volume 358, 2009 .Pages 137-146.
[4] R. Parr & W. Yang. Density Functional Theory of Atoms and Molecules. (Oxford University Press, New York, (1989).
[5] P . Chaquin (LCT UPMC) Pratiques de Chimie Theorique methodes fonctionnelles de la DFT.
[6] D. Singh, H. Krakauer, and C. S. Wang. Accelerating the convergence of self-consistent linearized augmented-plane-wave calculations Phys. Rev. B 34, 8391 – Published 15 December 1986.
[7] W. Kohn et L.J. Sham: Self-consistent equations including exchange and correlation.
[8] J. P. Perdew, Physica B172 (1991).
[9] J. Perdew, S. Burke and M. Ernzerhof.Phys. Rev. Lette77 (1996) 3865.
[10]T.L. Loucks, The Augmented Plane Wave Methode. Benjamine, New York(1967).
[11] Savrasov .S , Savrasov .D .Full potential linear Muffin-Tin in orbital method for calculating total energy and forces. Phys .Rev.B.46.121816-12195. 1992.
[12]Savrasov.S . Y. Linear response theory and lattice dynamics : a Muffin-Tin orbital approach . Phys .Rev.B.16470-6486. 1992.
[13] Savrasov SY. Linear-response theory and lattice dynamics: a muffin-tin-orbital approach, Physical Review B 54 (1996) 16470-16486.
[14]S. Y. Savrasov, Program LMTART for Electronic Structure Calculations, Zeitschrift für Kristallogr 220 (2005) 555-557.
[15] M. Born, K. Huang, Dynamical Theory of Crystal Lattices, Clarendon, Oxford (1956).

O-58

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Title: Green synthesis, characterization and antibacterial activity of eutectic mixtures of metronidazole

Farida ALLAL[a], Omar ElFarouk HOUACHE[a], Messouda BOUZIANI[a], Zohra HOUYOU[a]

[a] Mechanical Laboratory, Faculty of Sciences, Amar Telidji University, Laghouat, Algeria

Abstract:

This study aimed to improve the antibacterial activity of metronidazole (MTZ) by combining it with two amino acids as coformers. In this work, two pharmaceutical combinations of MTZ with L-arginine (ARG) and L-proline (PRO) were prepared by the liquid-assisted grinding method in a 1:1 molar ratio and characterized by differential scanning calorimetry (DSC) and Infrared spectroscopy. The thermal analysis revealed the existence of an endothermic event for the two binary mixtures investigated, at a temperature lower than the temperature of the pure components, characteristic of the formation of eutectic mixtures. The IR spectra of these eutectic mixtures revealed peaks corresponding to both MTZ and coformers. This result confirms the presence of the original crystalline state of the parent compounds in the binary pharmaceutical system, without the formation of new molecules or alterations in intermolecular interactions.

The antibacterial activity of the two eutectic mixtures obtained and the pure antibacterial agent was evaluated against aerobic and anaerobic bacterial strains. As a result, the two combinations displayed a synergistic effect. This phenomenon yields a significantly stronger therapeutic impact compared to the combined effect expected for the separately used substances.

Key words: Antibacterial drug, Arginine, Proline, Antibacterial activity

Corresponding Email:

f.allal@lagh-univ.dz

References

[1] S. A. Dingsdag and N. Hunter, "Metronidazole : an update on metabolism , structure – cytotoxicity and resistance mechanisms," no. October 2017, pp. 265–279, 2018, doi: 10.1093/jac/dkx351.

[2] A. Hernández Ceruelos, L. C. Romero-Quezada, J. C. Ruvalcaba Ledezma, and L. López Contreras, "Therapeutic uses of metronidazole and its side effects: An update,"

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Microbial fuel cell: a greener way to protect the environment

M. **A.Charef[a,b] , M.Kameche [b],B.Mohamed[b] , C.Innocent [c]**

[a]*Université hasiba benbouali chlef, Faculté technologie, département de tronc commun ,*
[b]*Université de science et technologie mohamed bodiaf oran,faculté de physique ,département de physique des matériaux ,laboratoire LPCMCE*
[c]*Université de Montpelier 2, institut européenne des membranes iem Montpelier France.*

Abstract:

The indiscriminate use of fossil fuels, coupled with overpopulation and pollution, has profoundly impacted the environment. To restore and maintain nature's balance while addressing energy scarcity, microbial fuel cells (MFCs) emerge as a green alternative. MFCs constitute an electrochemical system that converts biodegradable organic waste into electric energy through the activity of electrochemically active microorganisms.The MFC concept is in its early stages and holds vast unexplored potential. The system operates by converting organic substances into protons and recoverable electrons in the anode compartment. Electrons flow from the anode to the cathode through an external electrical circuit, engaging in reduction reactions. Concurrently, protons travel to the cathode through a glass bridge, facilitating reactions. At the cathode, electron and proton reactions with dissolved oxygen generate electricity, completing the system's circuit connected through a wire.MFCs also demonstrate the potential to reduce chemical oxygen demand and biological oxygen demand (BOD) in wastewater reservoirs. In this project, laboratory-generated and industrial wastewater served as feed. Soil samples from diverse drainage and crucial locations were collected for bacterial screening and population establishment. Initial experimentation involved Escherichia coli for electricity generation using graphite electrodes in a dual-chambered fuel cell.This innovative approach introduces alternative materials in lieu of traditional electrodes and catalysts, making MFCs a promising technology for cultivating a sustainable environment. The intersection of biology and electrochemistry in MFCs opens new avenues for harnessing energy while mitigating environmental impact.

Key words: MFCs, cathode, wastewater, protons.

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

International and National Efforts to Protect the Environment from Chemical Pollution Between Innovative and Traditional Mechanisms

Ben Hamid Abdelkader [1]

[1]Faculty of Law and Political Science

benhamid.abdelkader@yahoo.com

Abstract:

Pollution has expanded, becoming a global environmental phenomenon, occupying a significant portion of the world's attention since the 1960s. Over time, this phenomenon has generated serious environmental problems due to pollutants produced by industry and modern technology, usually accompanied by the production of hazardous materials that adversely affect the environment and its biological surroundings. Chemical pollution is one of the modern and dangerous phenomena that have affected environmental life and its elements such as seas, water, soil, air, humans, and animals due to industrial and technological developments and their misuse. This hastened the international community to make every effort at the international, regional, and national levels to mitigate this phenomenon by establishing legal mechanisms to protect the environment from the danger of chemical pollution, given the inadequacy of traditional mechanisms in addressing this phenomenon within the framework of achieving sustainable development.

Keywords: Environment and pollution, international efforts, chemical substances, innovative mechanisms, sustainable development.

Poster Communications

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Adsorption of Methyl Orange and Methylene Blue by a Biomaterial: Kinetic and Thermodynamic Study

DRA Rafik El Arslene [a], DRA Amira Ghislaine [b], MEDJAHDI Malika [a], RAMDANI Nadia[a]

[a] Departement of energy and process enginnering, DJILLALI LIABES University, Sidi Bel Abbes, Algeria
[b] Departement of Biology Sciences, DJILLALI LIABES University, Sidi Bel Abbes, Algeria

Abstract:

The aims of this study were the preparation of a powdered activated carbon obtained from jujube kernels to be applied as adsorbents in the removal of organic coloring contaminants from wastewater. Activated carbons were produced by a combination of chemical activation and pyrolysis processes. When applied as adsorbents in the removal of methylene blue (MB) and methyl orange (MO) from wastewater, the maximum removal values obtained from 1g of activated carbon obtained were achieved 93.86 % at pH = 6.28 (BM) and 90% at pH = 4 (MO). The adsorption results showed that the adsorption was faster at the beginning and reached its maximum around 120 min. The pseudo-second order kinetic model presents the best fit to the experimental data thus the adsorption of the two dyes is well suited to the LANGMUIR model with R^2=99.19% and Qm= 11.236mg/g for the case of BM and R^2=99.12% and Qm = 11.961mg/g for MO. The production of activated carbons from jujube kernels provides an effective adsorbent for the removal of the two cationic dyes (methylene blue and methyl orange).

Key words: Cationic dyes, Jujube cores, Adsorption, Activation carbon, Wastewater, kinetic.

Corresponding Email:
dra.rafik@gmail.com

P-002

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Title: synthesis and application of nickel nano-composite

Benouali Mohamed elamine[a], Beldjilali mohammed[a], boussalem smain[a]

[a]department of science of matter ; faculty of science and technology, laboratory of chemistry applied Bp284, university of Ain temouchent,46000,Ain temouchent ,Algeria

Abstract:

In this work sepiolite / nickel oxide (NiO) nano-composites were prepared by a green chemistry[1] and have been studied by various characterization techniques such as DRX and UV.

In the first part, NiO nanoparticles are synthesized in the presence of sepiolite in aqueous solution by the bio reduction of nickel sulfate with the extract of a medicinal plant. In the second part, the Nano-composites thus prepared are used as a catalytic support for the purification of water loaded with cationic dye (methylene blue). The influence of different parameters such as temperature, mass and contact time were studied[2]. The study of the kinetics as a function of concentration showed that the percentage removal of methylene blue increases as the mass of the catalyst increases. The values of $\Delta G°$ and $\Delta H°$ show that the degradation process studied is spontaneous and endothermic.

Key words: nanoparticule,depollution, extraction, sodium borohydride

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Elastic, magnetic and electronic behaviors of $EuFe_4P_{12}$ Filled-Skutterudite: DFT+U study

Z.A. Ziani, H. Bouafia

Physical Engineering Laboratory, University of Tiaret, 14000, Algeria.

Abstract:

Previous work has shown that $EuFe_4P_{12}$ has a Filled-Skutterudite structure that is stable in the ferromagnetic phase. Despite these results, several physical behaviors of this compound have not been studied to date, therefore, in our work, a comparative study of the structural properties has been carried out and the found results, of the structural parameters, are very close to the experimental comparison values. For the first time, in this work, a study of the elastic properties has been carried out, from which, the mechanical stability of $EuFe_4P_{12}$ has been confirmed and a detailed study of the elastic anisotropy has been carried out. Several mechanical quantities have been also estimated in this work such as Young's modulus, shear modulus and Poisson's ratio. The magnetic and electronic properties of $EuFe_4P_{12}$ are also the subject of this work, from where the obtained results have confirmed its ferromagnetic behavior that is mainly due to the contribution of the f-states of the europium atom. The work has been mainly carried out with FP-LAPW [1,2] method implemented in the WIEN2k code [3,4].

Keywords: $EuFe_4P_{12}$; Filled-skutterudites; FP-LAPW; ferromagnetic; elastic anisotropy.

Corresponding Email: zakariaabdelhafid.ziani@univ-tiaret.dz

References

[1] K. Schwarz, P. Blaha, G.K.H. Madsen, Comput. Phys. Commun. 147 (2002) 71.
[2] G.K.H. Madsen, P. Blaha, K. Schwarz, E. Sjöstedt, L. Nordström, Phys. Rev. B 64 (2001) 195134.
[3] P. Blaha, K. Schwarz, F. Tran, R. Laskowski, G.K.H. Madsen and L.D. Marks, J. Chem. Phys. 152 (2020) 074101.
[4] P. Blaha, K. Schwarz, G. K. H. Madsen, D. Kvasnicka, J. Luitz, R. Laskowski, F. Tran and L. D. Marks, WIEN2k, An Augmented Plane Wave + Local Orbitals Program for Calculating Crystal Properties (Karlheinz Schwarz, Techn. Universität Wien, Austria), 2018. ISBN 3-9501031-1-2. P.

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Elastic anisotropy and magnetic properties of CeNiSb Half-Heusler: First-principles investigation.

L. Messadi[a],H.Bouafia[a],B.Djebour[a],B.Sahli[a]

[a] Physical Engineering Laboratory, University of Tiaret, 14000, Algeria

Abstract:

CeNiSb is a ferromagnetic half-Heusler that has very fascinating physical properties. Several works have already exposed an important part of its physical behavior, while several others have not yet been studied. In our work, a complementary study is envisaged using the FP-LAPWmethod [1,2] (implemented in WIEN2k code [3,4]) which begins first with the study of the structural properties then the calculation of the elastic constants stiffness Cij. The latter can be exploited to study other new properties of this compound, notably elastic anisotropy. The latter is studied in detail by the theoretical model of J. Nordmann et al.[5,6]. Elastic anisotropy has been studied in detail and according to the different directions of space. This compound is ferromagnetic, which contains an atom belonging to transition metals with a partially filled 3d subshell, therefore, this indicates a presence of strong correlation between the electrons of this orbitals, which should be taken into consideration. The Ueff value (Hubbard's term) has been estimated by linear response method implemented in Quantum-Espresso code [7-9]. This correction has been added to GGA functional and a precise study of the electronic and magnetic behaviors has been carried out.

Key words: CeNiSb; FP-LAPW and PPs; ferromagnetic half-Heusler; Elastic anisotropy.

Corresponding Email:

(*):L. Messadi- Email : larbi.messadi@univ-tiaret.dz

P-005

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

The Impact of Emulsifier on (1:1) Metronidazole:Ethylcellulose Nanoparticles' Characteristics

Khalida MECHETTEM[1], *Zineb ELBAHRI*[2], *Kheira DIAF*[1]

[1] Laboratory of Macromolecular and Physical Organic Chemistry, Faculty of Exact Sciences, Djillali Liabes University of Sidi Bel Abbes, 22000 Sidi Bel Abbes, Algeria.
[2] Laboratory of Material and Catalysis, Faculty of Exact Sciences, Djillali Liabes University of Sidi Bel Abbes, 22000 Sidi Bel Abbes, Algeria.

Abstract:

Metronidazole is used to treat bacterial infections in different areas of the body. It is also used to treat infections caused by protozoa (eg, trichomoniasis and amebiasis) and infections caused by bacteria that do not need oxygen to survive. Since Metronidazole has a favorable solubility at a pH of 1.2, this study is aimed to elaborate polymer-based formulations with delayed release properties. This will allow to the colon drug release where the pH levels are 6.8 and 8.

The nanoparticles are prepared by microencapsulation process using water in oil emulsion-solvent evaporation technique where liquid paraffin is chosen as external phase. Ethylcellulose is used as polymeric matrix and the drug:polymer ratio is set at 1:1 and the emulsion is started with and without an emulsifier agent (Span 80). The selected variables are then the emulsifier concentration and the stirring speed of emulsion (800 and 1200 rpm).

The obtained formulations are characterized by infrared spectroscopy and X-Ray diffraction analysis and the size distribution of microparticles is determined by Zeta-sizer and the optical microscopy.

The drug release is studied in a simulated gastric liquid at pH=1.2 at 37°C and an intestinal medium (pH=6.8) and analyzed using UV-Vis spectrophotometer.

The drug loading varied from 44,86 to 54,89 % in these formulations. The results demonstrated that these systems allowed to a delayed drug release.

Key words: Metronidazole, nanospheres, drug release, emulsifier.

Email: mechettem.mechettem@yahool.fr

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Microporous Activated Carbon from wood waste and its Application in the Removal of Rhodamine B from Aqueous solution

Benzaidi Orkia[a], Aouatef Driouch[a], Yamina Benmerzouka[a], Aguedal Hakim[b], Sid Ahmed Ziat[a], Merouani Rhéda Djillali[a]

[a]Laboratory of Materials Valorization, Department of Process Engineering, Faculty of Science and Technology, Abdelhamid Ibn Badis University - Mostaganem, Bp. 227, 27000 Mostaganem, Algeria.

[b]Department of Preparatory Classes Higher School of Saharan Agriculture, Adrar, Algeria

Abstract:

In the present study, modified sawdust has been used as precursor for the preparation of activated carbon (MH300). using chemical activation method. The activated has been occur at low temperature (300°C) in air atmosphere[1] and at the impregnation ratio of 1:1 with H_3PO_4. The effect of various process parameters such as pH, initial dye concentration, adsorbent dose, contact time and temperature on the removal efficiency of Rhodamine B (RhB) was studied. Adsorption of (RhB) on MH300 was independent of pH. Optimum condition for adsorbent dose was determined to be 1.0 g/L. The time required to reach equilibrium depended on the initial dye concentration, being 240 min for the 10 mg/L concentration, 420 min for 25 mg/L and 1440 min for a concentration of 50 mg/L[2]. The adsorption equilibrium data were well explained by the Langmuir isotherm and Freundlich isotherm parameters, which suggested that RhB adsorption on the prepared MH300 was a physical adsorption. The kinetic data were better followed pseudo-second-order kinetics. The endothermic nature and randomness of the process were estimated from thermodynamic parameters. Based on the results obtained, it can be concluded that organic waste can be used as a low-cost biosorbent for dye removal in water treatment.

Key words: Adsorption; Activated carbon; Modified sawdust; Rhodamin B; Adsorption isotherm; Adsorption kinetics

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Structural, elastic, electronic and dynamical properties of $BaLiF_3$ Perovskite : Pseudopotentials study

B. Djebour, H.Bouafia, B.Sahli, L.Messadi, S.Mokrane

Physical Engineering Laboratory, Ibn Khaldoun University of Tiaret – Algeria.

Abstract:

The main objective of this work is to study the structural, elastic, electronic and dynamical properties of $BaLiF_3$ perovskite. Our calculations were carried out using the pseudopotentials method implemented in Quantum-Espresso code as part of the DFT [1-3]. Structural properties such as lattice parameter, bulk modulus and its pressure derivative were estimated and compared with previous results, good agreement was found [4,5]. The estimation of the elastic constants C_{11}, C_{12} and C_{44} made it possible to confirm the mechanical stability of this perovskite and other mechanical quantities were calculated [5]. The electronic properties are also the subject of this work, and the found results have made it possible to highlight the fascinating electronic character of this compound. Dynamical stability was studied by density functional perturbation theory (DFPT). The obtained results are in good agreement with the available comparison results [6,7].

Key words: PPsPW, DFT, perovskite, $BaLiF_3$, DFPT

Corresponding Email: benali.djebour@univ-tiaret.dz

References

[1] P. Giannozzi, et al., J. Phys. Condens. Matter 21 (2009) 395502.

[2] P. Giannozzi, et al., J. Phys. Condens. Matter 29 (2017) 465901.

[3] P. Giannozzi, et al., J. Chem. Phys. 152 (2020) 154105.

[4] Battal G Yalcin et al 2016 Mater. Res. Express 3 036301

P-008

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Structural and magnetic properties of $PrCrO_3$ and $PrVO_3$ magnetic perovskites: DFT+U study

H. Moussa , H. Bouafia

Physical Engineering Laboratory, University of Tiaret, 14000, Algeria

Abstract :

Magnetic Perovskites have attracted the attention of researchers in recent years due to their diverse and fascinating physical properties. Perovskites based on magnetic elements such as: PrCrO3, PrVO3, SrTiO3 and CaUO3 are known for their stability and magnetic properties which are mainly due to transition metals or rare earths. The aim of this work is to confirm the magnetic (ferromagnetic) and structural (cubic) phase of both PrCrO3 and PrVO3. Other physical properties are also considered such as the confirmation of their mechanical stability and their elastic behavior. The realization of this work is based on (FP-LAPW) method [1] within the framework of density functional theory (DFT) [2,3], which is implemented in WIEN2k code [3,4]. GGA functional has been chosen for the exchange-correlation potential [4]

keywords: Ferromagnetic, Perovskite, DFT, Structural stability, Electronic properties

Corresponding author:

(*):H.MOUSSA- Email : hanane.moussa@univ-tiaret.dz

References

[1] K. Schwarz, P. Blaha, G.K.H. Madsen, Comput. Phys. Commun. 147 (2002) 71.

[2] G.K.H. Madsen, P. Blaha, K. Schwarz, E. Sjöstedt, L. Nordström, Phys. Rev. B 64 (2001) 195134.

[3] P. Blaha, K. Schwarz, F. Tran, R. Laskowski, G.K.H. Madsen and L.D. Marks, J. Chem. Phys. 152 (2020) 074101.

[4] P. Blaha, K. Schwarz, G. K. H. Madsen, D. Kvasnicka, J. Luitz, R. Laskowski, F. Tran and L. D. Marks, WIEN2k, An Augmented Plane Wave + Local Orbitals Program for Calculating Crystal Properties (Karlheinz Schwarz, Techn. Universität Wien, Austria), 2018. ISBN 3-9501031-1-2.P.

P-009

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Title: **Ab-initio study of new conventional superconducting materials**

Chaimaa.MOHAMMED-KRARROUBI[1,2*], Mostefa. DJERMOUNI[1, 3], Asmaa.MOHAMMED- KRARROUBI[4], Lalia.MESSAOUDI[1,2], and Nadjet ZEGGAI[1,2]

[1] Laboratory of Computational Physics of Materials (LPCM), Djilali Liabès University of Sidi-Bel-Abbès,Algeria

[2] Department of Physics, Faculty of Science and Technology, Ahmed ZABANA University of Relizane,Algeria

[3] Department of Physics, Faculty of Exact Sciences, Djillali Liabès University of Sidi Bel-Abbès,Algeria

[4] Renewable energy research unit in the Saharan (URERMS) -CDER, Adrar ,Algeria

Abstract:

In science there are materials that conduct electricity without resistance under a transition temperature this phenomenon is called superconductivity, superconducting materials vary such as cuprates, pnictides [1] and hydrogen-rich compounds (called hydrides) [2].

SC hydrides have been well explained by the Bardeen-Cooper-Schrieffer (BCS) theory [3], where the SC is driven by a condensate of electron pairs, called Cooper pairs, due to electron-phonon interactions. Hydrogen is a good candidate for high-Tc SC according to Ashcroft [4]. Metallic hydrogen with light atomic mass is expected to have high vibrational frequencies, thus providing high Tc through electron-phonon coupling (EPC) therefore metallization of hydrogen is very difficult to achieve experimentally, as it requires pressures too high above 400 GPa [5-6]. While in 2004 experimenters can perform SCs in hydrides at relatively lower pressures that are currently accessible using static compression techniques [7]. Experiments have been performed to confirm that sulfur hydride compressed H3S exhibits a Tc of 203 K at pressures around 150 GPa [8]. The objective of this work to know the microscopic mechanism of superconducting hydride materials in the first place, then to contribute to the exploration of new SC hydrides at high pressure. And in order to achieve our goals, we will use a first-principle method based on DFT theory. This theory helps us to predict the electronic, chemical, and phononic properties of hydride materials.

Key words: Materials Hydrides, Superconductivity, DFT, TC, electronic properties.

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Modification and characterization of activated carbon using magnetic(Fe3O4) and ZnO nanoparticles

OUALI Asmaa , Attouti Salima, Baghdad Benabed Fatma, Maiti chaimaa and khalili khadidja

Abstract

Nanotechnology is currently one of the most recent subjects, widely employed in various fields, particularly in chemical processes dedicated to environmental protection and the destruction of pollutants with adsorption being one of them. In our present study, we are going to apply this technology by synthesizing nanoparticles through co-precipitation method of Fe3O4 and ZnO using them to modify activated carbon's surface ; which is the most widely used adsorbent due to its cost and efficiency. We conducted two characterizations to gain insights into the surfaces of micro and mesopores in our synthesized carbons. These characterizations include the methylene blue index, with values of 237.13 mg/g for PAC, 296.39 mg/g for PAC/Fe3O4, and 297.32 mg/g for PAC/Fe3O4/ZnO. Additionally, the iodine values are 908.7 mg/g, 564.1 mg/g, and 548.65 mg/g for PAC, PAC/Fe3O4, and PAC/Fe3O4/ZnO, respectively.

Keywords: Powdered activated carbon(PAC), nanoparticle, iodine value, methylene blue index, PAC/Fe3O4, PAC/Fe03O4/ZnO

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Advancements in Fuel-Rich Propellants: An In-depth Exploration of Boron Coreshell with Sodium Azide for Enhanced Combustion Efficiency in Propulsion Systems

Mohammed el amine FACIH [1, a] , Moulai Karim BOULKADID [1,b] , Sabri TOUIDJINE[1, c] * and Samir BELKHIRI [1,d]

Abstract

Fuel-rich solid propellants, characterized by an excess of fuel relative to the oxidizer, play vital roles in various propulsion systems, including rocket motors, engines, and pyrotechnic devices. Their ability to deliver high energy output makes them indispensable in aerospace and related industries. This study focuses on enhancing fuel-rich propellants by incorporating boron and boron modified with sodium azide. The challenges associated with boron's combustion efficiency, such as high ignition points and oxide film formation, are addressed. The research explores the novel approach of using sodium azide as a coating for boron in propellant formulation. The synthesized propellants (SCPs) based on boron and boron modified with sodium azide undergo thorough characterization for physico-chemical and thermal attributes, including FTIR, RAMAN, X-ray diffraction (XRD), bomb calorimetry, thermogravimetric analysis (TGA), and differential scanning calorimetry (DSC). Simultaneously, a comprehensive kinetic analysis is performed using iso-conversional methods, notably Iterative Kissinger-Akahira-Sunose (It-KAS) and Flynn-Wall-Ozawa (It-FWO). Combustion tests provide valuable insights into the propellants' performance. This work contributes to the advancement of efficient propulsion systems, particularly in the context of ducted rockets.

Keywords: Fuel-rich solid propellants, modified boron, Energetic Performance, kinetic analysis.

P-012

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Title: Spinel ferrite nanoparticles-graphene oxide nano-composite: synthesis and its catalytic effect on the thermal behavior of nitrocellulose-based mixture

LOUAFI Elamine[a], Moulai Karim BOULKADID[a], TOUIDJINE Sabri[a]

[a] Energetic Propulsion Laboratory, Teaching and Research unit of Energetic Processes, Ecole Militaire Polytechnique, BP 17, Bordj El-Bahri, 16046, Algiers, Algeria.

Abstract:

Our study explored the catalytic properties of nanocomposites of spinel ferrite nanoparticles (SFN) with graphene oxide (GO) in the thermal decomposition of a NitroCellulose-Based mixture (NCB). The synthesized samples, upon incorporation into the NCB formulation, underwent thorough analysis using spectroscopic techniques, including FT-IR and Raman spectroscopy. Differential scanning calorimetry (DSC) was employed to explore the impact of the prepared catalyst on the thermal degradation of NCB. The non-isothermal kinetic parameters, determined through Iterative Kissinger–Akahira–Sunose (It–KAS), Vyazovkin's nonlinear integral with compensating effect (VYA/CE), and Iterative Flynn–Wall–Ozawa (It–FWO) techniques, revealed a significant reduction in the activation energy barrier for NCB catalyzed by 3% of MFe_2O_4@GO (M= Co, Cu), approximately of 20%. This suggests the promising catalytic potential of the synthesized materials for enhancing the thermal decomposition efficiency of double-base propellants.

Key words: Nitrocellulose, spinel ferrites, graphene oxide, nanocomposite, kinetics, thermal decomposition.

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Study of chemical composition and biological activity of differents plants

Chaimaa Kalache [a], Assia Keniche[b], Yasmine Soltani[b], Amina Aboura[b], Fatoumata Samaké, Zoheir Arrar[b], Mohammed El Amine Dib[b], Okkacha Bensaid[b]

[a]Department of chemistry, Faculty of science, University: Abou Bakr Belkaid Tlemcen, Country: Algeria,
[b]Laboratory of Organic Chemistry Natural Products and Analysis, University of Tlemcen, Algeria

Abstract:

Medicinal plants are a precious heritage and a real treasure for humanity, they are in high demand in the world. They have been used for millennia to treat all types of pathologies. They are now attracting renewed interest as a therapeutic alternative to drug treatments.

The purpose of our research was to evaluate the antioxidant and antimicrobial activities of Moringa oleifera from Mali and Algeria, and also to determine the flavonoids and polyphenol content. Moringa oleifera is a highly cultivated plant in the Moringaceae family due to its many therapeutic benefits and health benefits. This plant is known for its numerous therapeutic virtues and health benefits. It is originally from South Asia, but it is now being grown in numerous tropical and subtropical regions around the world because it is becoming increasingly popular as a medicinal and nutritional plant. The study aimed to determine the total amount of polyphenols and flavonoids in an extract of Moringa oleifera leaves, evaluate its antioxidant activity using two methods (DPPH and FRAP), and measure its antimicrobial activity against selected bacteria. The study's results revealed that Moringa oleifera leaves contain high levels of flavonoids and polyphenols. The antioxidant properties of these compounds suggest that Moringa oleifera leaves could be a useful tool in fighting oxidative damage in the body. Furthermore, the study showed that the extract of Moringa oleifera leaves from Mali exhibited the best antioxidant activity according to both methods (DPPH and FRAP), highlighting its effectiveness as an antioxidant agent. Regarding antimicrobial

activity, extracts of Moringa oleifera leaves were tested against various bacterial strains, including E. coli, P. aeruginosa, K. pneumoniae, B. subtilis, and S. aureus. The results indicated that Moringa oleifera leaves from Mali exhibited the highest antimicrobial activity among the tested samples. These findings suggest that Moringa oleifera leaves, especially those from Mali, are rich in antioxidant compounds, flavonoids, and polyphenols, which may contribute to their potential therapeutic benefits. The antimicrobial properties of these compounds against multiple bacterial strains make them essential for medical research and healthcare.

Key words: Moringa Oleifera, Flavonoids, Polyphenols, Activity, Antioxidant, Antimicrobial.

Corresponding Email: kalache.ch@hotmail.com

References

[1] Singh, Navneet; Ethnomedicinal Pharmacological and Antimicrobial Aspects of Moringa oleifera Lam.; Review *the journal of pharmacology ;* **2018*;*** **,**45-50.

[2] Bourai, guelmani-ziani; Antioxidant activity of seed extracts of nutritional and medicinal interest: Moringa oleifera; A. MIRA University – Bejaia; Master thesis 2015 page16.

[3] Vergara, J.M.; Almatrafi, M.M.; Fernandez, M. L.; Bioactive Components in Moringa Oleifera Leaves Protect against Chronic Disease, *Review antioxidants MDPI,* **2017**, 6, 1-13.

P-014

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Elaboration de Nanoparticules Mésoporeuses et Dégradation par Ozonolyse du Diclofenac de Sodium

Chaimaa Maiti[a], Mourad Termoul[a], Salima Attouti[a], Benaouda Bestani[a], R.ouargli Saker[a]

[a]Laboratoire de Structure, Elaboration et Application des Matériaux Moléculaires (SEA2M), Faculté des Sciences et de la Technologie, Université Abdelhamid Ibn Badis-Mostaganem, Algerie.

Résumé:

La dégradation de notre environnement et les perturbations que subisse notre écosystème suite à la pollution avec les différentes formes et sources font partie des sujets d'actualités et présentent une préoccupation mondiale. L'industrie pharmaceutique fait partie des secteurs pointés du doigt dans cette crise écologique. En effet, la présence d'une grande variété de composés pharmaceutiques, tels que les antibiotiques, les analgésiques, les anti-inflammatoire. L'élimination de ces polluants de notre environnement est primordiale, face aux méthodes de traitement conventionnel peu efficace, la dégradation par ozonolyse catalysée représente une grande opportunité. Dans ce travail nous avons élaboré deux matériaux mésoporeux avec deux structures cristallines différentes. La SBA-15(Santa Barbara Amorphos) de structure hexagonale et la SBA-16 de structure cubique en vue d'améliorer l'activité catalytique de ces deux matériaux. Nous avons optés pour une modification par le greffage d'une molécule organique de type 3-phenyl-4-benzoyl-5-isoxazolone (HPBI) de caractère acide. Afin d'obtenir des catalyseurs bifonctionnels, après nous avons élaboré des nanoparticules mésoporeuses par l'insertion du métal de fer sur les matériaux greffés par la HPBI. La caractérisation des matériaux par diverses méthodes d'analyse tels que DRX, analyse gravimétrique (ATG) et adsorption/désorption de l'azote à 77K, les caractérisations nous a permis de mettre en évidence les changements de leurs structure et morphologie par suite du la méthode de préparation appliquée. La porosité et l'aire spécifique sont considérablement développées. Par ailleurs, le traitement thermique conduit à un matériau essentiellement mésoporeux. Les matériaux fonctionnalisés obtenus de nanoparticules de fer de charge zéro ont été testés par la suite dans la dégradation par ozonolyse catalysé du Diclofénac de Sodium. Quelques facteurs (temps de contact, pH, concentration du diclofénac de sodium) affectant les équilibres de dégradation ont également été étudiés. L'ozonation catalysée par les matériaux fonctionnalisés Fe-HPBI-SBA-15 et Fe-HPBI-SBA-16 a été considérée nécessaire pour la minéralisation totale du Diclofénac de Sodium.

Mots clés : catalyseurs, nanopaticules mésoporeuses, Diclofénac de Sodium, dégradation.

P-015

ICMSE'2024

Study of structural and electronic properties of Perovskite $SrMoO_3$ using FP-LAPW method

S. Mokrane [a, b], *B. Djebour* [b]

[a] *Department of Physics, the Higher Normal School of Mostaganem*

[b] *Laboratoire de Génie Physique, Université Ibn Khaldoun, Tiaret 14000, Algeria*

Abstract:

In this work, we present the electronic properties of perovskite $SrMoO_3$ by using the full potential linearized augmented plane wave (FP-LAPW)[1] method. The densities of states and energy band structures have been calculated by using the generalized gradient approximation (GGA)[2] as exchange-correlation potential.

The results obtained are in agreement with the previous experimental and theoretical results. The obtained value of energy band gap of 3.8 eV.

Key words: FP-LAPW, perovskite, DFT, GGA.

Corresponding Email:
Mokranesetti585@gmail.com

References

[1] P. Blaha, K. Schwarz, P. Sorantin, S.B. Trickey, Full-potential, linearized augmented plane wave programs for crystalline systems, Comput. Phys. Commun. 59 (1990) 399.

[2] J.P. Perdew, K. Burke, M. Ernzerhof, Generalized gradient approximation made simple, Phys. Rev. Lett. 77 (1996) 3865.

P-016

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Preparation of a Novel Membrane of Poly (4-Chlorostyrene) clay composite, by cationic polymerization of p-Chlorostyrene using green catalysis

Ait Amer Ahcene [a,b], Chadli Redouane [a,c], Boukriris Sadia[b], Benaddane Kaddour [a]

[a] Department of Chemistry, Faculty of Exact Sciences, University of Djillali Liabes of Sidi Bel Abbes (UDL). BP 89, 22000 Sidi Bel Abbes. Algeria.
[b]Laboratory of Chemistry and Electrochemistry of the Metallic Complexes (LCECM), University of the Sciences and Technology of Oran-Mohamed Boudiaf (USTO-MB), Oran, Algeria.
[c] Laboratoire de Chimie Organique Physique et Macromoléculaire (LCOPM) University of Djillali Liabes of Sidi Bel Abbes (UDL). BP 89, 22000 Sidi Bel Abbes. Algeria.

Abstract:

In recent years, technical advanced and knowledge of green catalytic materials draw much interest and attention to develop new ways to prepare thermoplastic materials at a lower cost and respecting the environment. In the current work poly(p-chlorostyrene) clay composite was prepared [1-3]. Cationic polymerization of Cl-Styrene using a natural clay called Maghnite-H^+ as catalyst was carried out, under mild synthesis conditions: in bulk and at room temperature according to the principles of green chemistry [4-5]. Effects of Cl-St molar ratio, catalyst concentration were studied. The structure of the product obtained was confirmed by ^{1}H-NMR, ^{13}C-NMR (nuclear magnetic resonance), infrared spectroscopy (IRFT) and thermogravimetric analysis (TGA) for thermal properties of the resulting polymer. Comparison with two other conventional catalysts, namely $SnCl_4$ and PBO, was established.

Key words: Poly(p-chlorostyrene) PCS, composite clay, membrane, green catalysis

Corresponding Email: aitamer.ahcene9@gmail.com

References

[1] Kausar. A, Research, Journal of Nanoscience and Engineering, V2, Issue 1, (2018), 28-33
[2] Li, YQ., Zhou, J., Xiao, R. et al. Chin J Polym Sci 38, 941–949 (2020).
[3] Purohit P, Bhatt A, Mittal RK, Abdellattif MH and Farghaly TA (2023), Front. Bioeng. Biotechnol. 10:1044927. doi: 10.3389/fbioe.2022.1044927
[4] M .Belbachir, A. Bensaoula, Composition and Method for Catalysis using Bentonite, US Patent N° 7,094,823 B2, (2006).
[5] M. I. Ferrahi, A. Ait Amer, M. Belbachir, A. Benyoucef, E. Morallon . Organic Chemistry- Indian journal, 2 (2006)165-169.

P-017

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Extraction of biopolymers from sheep's wool and their environmental preservation

Karima OUSSADI

Université des Sciences et de Technologie Mohamed Boudiaf. Laboratoire de Physico-Chimie des Matériaux Catalyse et Environnement (LPMCCE), BP 1505, Oran, ALGERIE

Abstract:

This work falls within the framework of environmental preservation, economic growth and waste recovery based on green chemistry and biopolymers from biomass. Herein we present the extraction of keratin and lanolin from the sheep's wool in green chemistry conditions and having characteristics that allow them to be effective for the environment. Spectroscopy including FT-IR and MEB were used to elucidate structural characteristics of the resulting products of the extraction. Wool is a product of nature, it is formed in sheepskin. It is built from a protein called keratin which is formed in the process of alpha-amino acid biosynthesis. It contains up to 95% pure keratin by weight[1]. Keratin is a biopolymer with a high degree of chemical functionality and exhibits many properties that synthetic polymers cannot achieve. Process of extraction of keratin is cited in many papers[2,3,4]. Lanolin is the product obtained after purification of wool fat secreted by the sebaceous glands.

Key words: Environment, Biomass, Biopolymer, Extraction, Keratin, Lanolin, Wool.

Corresponding Email: : karima.univchimie@gmail.com

[1] P. V. Peplow, A.D. Rodick-Lanzilotta, United states Patent 2005/0232963 A1, **2005**.
[2] J. M. Cardamone.; A. Nunez.; R. Garcia.; R. M. Aldema-Ramos. Res. *Lett. Mater. Sci*. **2009.**
[3] J. M. Cardamone.; J. G. Phillips. *Textile Res. J. 5*, 277-283. **2007.**
[4] J. M. Cardamone. *Journal of Molecular Structure. 968*, 97-105. **2010.**

P-018

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Advancements in Fuel-Rich Propellants: An In-depth Exploration of Boron Coreshell with Sodium Azide for Enhanced Combustion Efficiency in Propulsion Systems

M. Khelil [a, b]*, M. Guemou [c], A. Ammari [d, e], B. Abbar [f], A. Abdiche [g], R. Moussa [h]

a) Department of Physics, Djillali Liabès University, Sidi-Bel-Abbes (Algeria).
b) b) Laboratory of Industrial Technology, Ibn Khaldoun University, Tiaret (Algeria).
c) c) Department of Sciences and Technology, Ibn Khaldoun University, Tiaret (Algeria).
d) d) Department of Physics, Faculty of Matter Sciences, Ibn Khaldoun University, Tiaret (Algeria).
e) e) Laboratory of Micro and Nanophysics, National Polytechnic School (ENPO),Oran (Algeria).
f) f) Computational Materials Science Laboratory, Djillali Liabès University, Sidi-Bel-Abbes (Algeria).
g) g) Applied Materials Laboratory, Djillali Liabès University, Sidi-Bel-Abbes (Algeria).
h) h) Physics Department, University Ziane Achour, Djelfa (Algeria)

Abstract

The triangular quaternary system BxIn1-xNyAs1-y represents a promising class of materials with tunable physical properties due to the combination of boron, indium, nitrogen, and arsenic. By varying the composition (x and y), one can achieve a wide range of band gaps (0.12 to 2.10 eV), electrical conductivities, and optical absorption coefficients, making them suitable for various applications such as photovoltaic, light-emitting diodes (LEDs), and thermoelectric. The ongoing research and development efforts in the field of BxIn1-xNyAs1-y materials hold immense promise for the future of optoelectronics, electronics, and other emerging technologies. BxIn1-xNyAs1-y adopts a chalcopyrite structure (space group I-42d), similar to chalcopyrite minerals like $CuFeS_2$. In this structure, cations (B-In-N) occupy the tetrahedral sites in a face-centered cubic lattice, while anions (As) occupy the octahedral sites. Varying the composition (x and y) can lead to lattice distortions (a=4.59 to 5.77 u.a) and changes in bond lengths and angles, impacting the material's properties. These structures can be broadly classified into Zinc blende-type and Wurtzite type. The band structure of BxIn1-xNyAs1-y compounds can be significantly altered by varying the composition (x and y). This allows for precise control over their electrical and optical properties, such as band gap Tuning.

Keywords: triangular quaternary; BxIn1-xNyAs1-y; ab-initio approaches; semi-conductor

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

matériaux composites à fibre végétale

Rahla Miloud , Deghfel Nadir , AZZEDINE BENYAHIA

Abstract

Le remplacement des fibres synthétiques par des fibres naturelles de cellulose engendre un Intérêt La biomasse, riche en cellulose, joue un rôle crucial en tant que matière première pour l'industrie chimique en raison de ses groupements fonctionnels adaptés au traitement chimique. Les fibres cellulosiques suscitent un intérêt croissant en raison de leur coût abordable, de leur légèreté [1], de leur biodégradabilité, de leur disponibilité et de leur capacité à être recyclées. Les matériaux composites renforcés par ces fibres trouvent des applications dans des secteurs exigeant des structures légères, robustes, rigides et résistantes à diverses contraintes, tels que l'aérospatiale, l'automobile, l'électronique, le pétrole et la médecine [2].

P-020

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Prédiction des propriétés structurales , élastiques et électroniques de la pérovskite CaTaO3 .

B.Sana [1], H. Bouafia [1], H. Moussa[1], S.Mokrane[1]

Abstract

L'objectif de ce travail a été développé une compréhension à l'échelle atomique des propriétés structurales, élastiques, électroniques des pérovskites « Exp:CaTaO3 », une classe de matériaux très prometteurs pour la réalisation de nouveaux dispositifs multifonctionnels. Nous avons utilisé les calculs de la théorie fonctionnelle de la densité (DFT) selon les principes de base pour développer cette compréhension. La méthode FP-(L) APW+lo telle qu'implémentée dans le code WIEN2k est majoritairement utilisée dans la réalisation de ce travail.

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Ab initio study of the structural, electronic and optical properties of BSb and BN compounds and their superlattices

Belghoul Hafida[a], Oukli Mimouna[a]

[a]Applied Materials Laboratory (A.M.L), Faculte de Genie Electrique, ´ University Djillali Liabes of Sidi Bel Abbes, 2200 Sidi Bel Abbes Algeria

Abstract:

In this study, the properties of boron compounds are investigated through a first-principles analysis, focusing on its structural, electronic, and optical properties. To create a zinc-blende superlattice with a (001) orientation, an ultrathin BSb layer is inserted into the BN structure. The full potential linear muffin-tin orbitals method (FPLMTO) incorporated in the LMTART computer code, using Perdew and al parameterization within the generalized gradient approximation (GGA96), is utilized for this analysis. The results of the electronic structure analysis confirm that these compounds exhibit semiconductor behavior along the (001) axis. The influence of the number of periodic layers (n) on the band gaps and optical activity of (BSb)/(BN)n superlattices in the (001) growth axis is examined and compared. Additionally, the analysis of the partial density of states reveals the significant impact of nitrided materials, such as BN, which can be attributed to the strong sp hybridization of N atoms.

Key words: Boron compounds, Superlattices, Electronic structure, optical ptoperties.

Corresponding Email:

hafidabelghoul@gmail.com

References

[1] R.M. Wentzcovitch, M.L. Cohen, P.K. Lam, Phys. Rev. B 36 (1987) 6058.

[2] E. Kim, C.F. Chen, Phys. Lett. A 319 (2003) 384.

[3] M. Guemou a,n, A.Abdiche b, R.Riane b, R.Khenata c PhysicaB436(2014)33–40

[4] E. Knittle, R.M. Wentzcovitch, R. Jeanloz, M.L. Cohen, Nature (Lond.) 337 (1989) 349

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Simulation of the energy of graphene nanoribbons by the DFT method with the SIESTA code

ZOUBIR BENKHANOUCHE[a], KHALED BOUFALA[b]

[a]* Department of Physics/Laboratory of Physical Chemistry of Materials and Catalysis, University of Bejaia, Algeria

[b]* Department of Physics/Laboratory of Physical Chemistry of Materials and Catalysis, University of Bejaia, Algeria

Abstract:

Graphene [1] is a nano-scientific material. It is a two-dimensional material made of a single layer of carbon atoms arranged in hexagons. It has important physical properties. This material is used in several applications and mainly in electronic junctions at the nanometric scale and in spintronics. Graphene-based nanoribbons are materials developed very recently with fascinating physical properties (electronic, electrical and magnetic) compared to the bulk state or that of graphene. In this study, we simulated these systems by siesta code. The study of the adsorption and doping [2] of these systems by transition metal atoms is justified by the stability of the ribbon-MT structures and by the catalytic power of the MT atoms on the surface which are likely to bind easily with other molecules. In this work, we carried out a study on the electronic, structural and magnetic properties of carbon nanoribbons adsorbed and doped by MT atoms. The objective was to see the effect of MT atoms on the geometric structure, electronic and magnetic of the nanoribbon. The calculations were performed by the ab-initio siesta [3,4] code within the framework of density functional theory DFT. It is a pseudopotential code that uses a digitized atomic orbital basis. The exchange-correlation term was treated by the generalized gradient approximation. We used the conjugate gradient method for the relaxation of structures. The results obtained show a change in the electronic, structural and magnetic properties.

ICMSE'2024

Developing a novel model for replicating the electric discharge phenomenon in the rod-plane air gap system

Benharat Samira[1], Belgacem Leila[2], Doufene Dyhia[3], Sakmeche Mounir[4]
[1,2]Research Centre in Industrial technologies – CRTI- Cheraga-Algiers - Algeria
[3]Department of Electrical Engineering, Electrical and Industrial System Laboratory (LSEI) , University of Science and Technology Houari Boumediene , Bab Ezzouar, Algeria
[4]Laboratory of Catalytic Materials and Industrial Processes (LMPCI), Department of hydrocarbons and renewable energies, Faculty of Science and Technology. University of Adrar, National High way No. 06. Adrar 01000, Algeria

Abstract- The current study introduces a novel approach to simulate electric discharges within a rod-barrier-plane air gap system. This model specifically accounts for the presence of insulating barriers. It's noted that the characteristics of the electrical discharge are influenced not only by the dimensions (thickness and width) of the insulating barriers but also by their positions within the air gap. Emphasis is placed on the significant role of the applied voltage mode. In this proposed model, AC voltage is considered for silicone rubber insulating barriers. Experimental findings indicate that the resulting arc can manifest across 1 to 4 channels. The discharges generated under AC voltage exhibit a distinctive multiple-channel arc formation. The developed model accurately replicates the discharge patterns observed in experimental tests conducted under AC voltage. It further validates that the electric field plays a crucial role in the behavior of the rod-insulating barrier-plane system.

Keywords: Insulator; Lightning; FEMM; Rod-insulating barrier -plane system; Silicone rubber barrière.

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

High-efficiency thermoelectric converter material: First-principles calculations of KBiBa half-Heusler compound .

Z. F. Meghoufel[1], A. Boukra[1], F. Mahi[1,2], I. Kara[1], Z. Mostefa[1,2]

Abstract

First-principles calculations, using the full potential approximation implanted in the WIEN2K code, and semi-classical Boltzmann transport theory implanted in the BoltzTrap code, were used to investigate electronic and thermoelectric properties of KBiBa Half-Heusler compound. The approximations used here such as TB-mBJ potential and spin-orbit coupling (SOC) show a semiconducting behavior of the compound with an indirect bandgap of 0.88 eV. By examining phonons' frequencies dispersion curves, no negative frequency is observed; Thus, the material is dynamically stable. The calculated elastic parameters meet the stability criteria of Born, proving the mechanical stability of the compound. Both stability conditions can conclude on the possible manifacture of the studied compound. By carrying out calculations on lattice thermal conductivity, effective mass of both electrons and holes of the compound and their respective relaxation times, and by using the deformation potential theory given by Bardeen and Shokley, we obtain the figure of merit ZT according to temperature and doping concentration in both charge carriers type. The figure of merit ZT in KBiBa reaches a value of 2.68 at 1200 K and n-doping concentration of 2.2 1019 cm-3, making it a good candidate for a high-temperature thermoelectric (TE) conversion, significantly reducing the energy lost by Joule effect.

Keywords Half-Heusler, thermoelectric properties, first-principles, spin-orbit coupling, figure of merit, deformation energy.

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Highly efficient removal of industrial dye under neutral conditions by UV photocatalysis process using novel TiO_2/Fe diatomite composite

Walid Rezig [a], Mohammed Hadjel [b]

[a] Laboratory of Sciences, Technology and Process Engineering LSTPE ; Department of Chemical Engineering ; Faculty of Chemistry ; University of Sciences and the Technology of Oran Mohamed Boudiaf USTO-MB ; BP 1505 El M'naoueur Bir El Djir 31000 Oran ; Algeria.

[b] Laboratory of Sciences, Technology and Process Engineering LSTPE ; Department of Physical Chemistry ; Faculty of Chemistry ; University of Sciences and the Technology of Oran Mohamed Boudiaf USTO-MB ; BP 1505 El M'naoueur Bir El Djir 31000 Oran ; Algeria.

Abstract:

A composite catalyst, termed "TDF" (titanium prepared ferric diatomite modified), was synthesized and characterized in this study. The TDF was created through surface modification treatments, which involved the deposition of $Fe(NO_3)_3 \cdot 9H_2O$ and TiO_2 Degussa P25 onto raw diatomite. During the $Fe(NO_3)_3 \cdot 9H_2O$ treatment, the surface silica of diatomite and TiO_2 Degussa P25 were partially dissolved. This modification process was investigated using various analytical techniques including X-ray fluorescence (XRF), scanning electron microscopy (SEM), thermogravimetric analysis (TGA), differential scanning calorimetry (DSC), and UV-visible diffuse reflectance spectroscopy (DRS). The surface area of the resulting TDF was measured to be 855 m^2/g. Furthermore, the modification increased the point of zero charge (pH_{PZC}) value to 6. The energy gap (Eg) of TDF was determined to be 1.1 eV using UV-visible DRS technique. The degradation of vat green 03 indanthren textile dye showed a pH dependency, with the most effective removal observed at pH=10, achieving a color removal of approximately 92 %. The photodecolorization rate followed a pseudo-first order kinetic with respect to the dye concentration.

Key words: titanium, ferric, diatomite, photodecolorization ,dye.

P-026

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Title: First-principles studies of novel lead-free halide double perovskite

KHATIR Radja[a,b], BLAHA Lamia Farah[c], AMERI Ibrahim[c], KESSAIRI Khadra[a]

[a]Laboratory of Electrical Engineering and Materials (LGEM), The Higher School of Electrical and Energetic Engineering (ESGEE), Oran, Algeria.
[b]Materials and Sustainable Development Department (LMCDD), Faculty of Science, University of Sidi-Bel-Abbes, Sidi-Bel-Abbes, 22000, Algeria
[c]Laboratory of Physical Chemistry of Advanced Materials (LPCMA), University of Djillali Liabes, Sidi-Bel-Abbes, Algeria

Abstract:

The structural, elastic, mechanical, and thermoelectric properties of Cs2AgFeCl6 lead-free halide double perovskite have been extracted and explored by a cohesive analysis using spinpolarized Density Functional Theory (DFT) associated with Boltzmann transport scheme. The exchange-correlation potential is determined through the generalized gradient approximation (GGA) and modified Becke-Johnson (mBJ). It is crystallized into cubic structure of ferromagnetic phase. The lattice parameter is estimated to be close to experimental data. The Cs2AgFeCl6 illustrates p-type ferromagnetic semiconducting properties. The 5 μB is estimated to have total magnetic moment with a necessary contribution for Fe atoms. The elastic properties prove that Cs2AgFeCl6 is stable and ductile. The thermoelectric properties of Cs2AgFeCl6 utilizing equations of Boltzmann transport through DFT into range, 100–900 K are calculated. According to our findings, it is demonstrated that Cs2AgFeCl6 is a promising candidate for thermoelectric applications at both high and low temperatures.

Key words: DFT , Lead-free double perovskites , Elastic Mechanical

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Study of the characteristics of the p+ emitters Produced during the metallization of the rear surface of n-type silicon solar cells .

Korichi H 1, Bensdira A 2, abdelghani B 3, Mohamed K 4

Abstract

Aluminium screen printing metallisation is widely used in the photovoltaic industry to form the backside surface field (BSF) in p-type cells. Recently, there has been a growing interest in n type cells with a p+ emitter on the backside realised by aluminium diffusion. This concept offers advantages in terms of industrial manufacturing.

Keywords: silicon, diffusion, emitter, metallisation, screen printing, solar cells

P-028

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Title: **Optical and bonding properties of hybrid metal-halide CH3NH3PbX3 (X = Br) perovskite: A density-functional theory study**

Presenting author's Amina Dendane[a], Benali Rerbal , Tarik Ouahrani …

[a]Amina Dendane ;[b] Benali Rerbal Département of physique , Laboratory of Materials Discovery, Unit of Research Materials and Renewable Energies, LEPM-URMER, University of Tlemcen 13000, Algeria

[c] Tarik Ouahrani Department, of physique theoretical laboratory ,university of Tlemcen 13000,Algeria

Abstract:

Organic-inorganic hybrid perovskites, such as lead halide MAPbX3 (MA= CH3NH3; X= Br), have generated significant interest in the field of energy materials. These materials exhibit a complex structure and adjustable properties and their wide range of light absorption, covering the visible and ultraviolet regions, makes them attractive for optoelectronic devices and photovoltaic applications. Hybrid perovskite solar cells have emerged as an exciting technology, enabling the fabrication of light-harvesting materials for efficient solar cells.
In this study, we employed the ab initio pseudopotential method implemented in the VASP code to analyze the electronic and optical properties of MAPbX3 perovskites. We have investigated the band structure, density of states, and optical absorption spectra of the hybrid perovskite materials. The results shed light on the fundamental electronic and optical characteristics that contribute to their potential as energy materials.
Overall, our findings highlight the significant advancements made in understanding the electronic and optical properties of hybrid perovskites. This knowledge contributes to the development of efficient photovoltaic and optoelectronic devices, paving the way for advancements in renewable energy and electronic technologies.

Key words: hybrid perovskites, solar cell, vasp code, optical properties

P-029

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

MEASUREMENT OF SILICON NITRIDE THIN FILM THERMAL CONDUCTIVITY USING THE 3-OMEGA METHOD

Amine Abdelkader Guermoudi [a,b], Pierre-Yves Cresson[c], Katir Ziouche[c], Amaria Ouldabbas[b], Tuami Lasri [c]

[a] Hassiba Benbouali University of Chlef, Chlef, Algeria.
[b] Renewable Materials and Energies Research Unit (URMER) / Aboubekr Belkaid University of Tlemcen, Tlemcen, Algeria.
[c] Institut d'Électronique de Microélectronique et de Nanotechnologie (IEMN) / Univ. Lille CNRS, Centrale Lille, ISEN, Univ. Valenciennes, Lille, France.

Abstract:

Silicon nitride (Si_3N_4) is a material widely used in the field of microelectronics, as an electrical insulator and chemical barrier in the manufacture of integrated circuits (transistors), in order to electrically isolate different structures or as an etching mask in mass micro-machining. In aerospace, it has been identified as one of the rare monolithic ceramic materials capable of withstanding thermal shock and extremely high temperature gradients from rocket engines (NASA) [1]. In medicine, it has also been used for spinal fusion devices [2,3]. Knowledge of the thermal properties, in particular the thermal conductivity, in thin films and thin film multilayer structures of this material is essential to optimize the performance of many devices. In this paper, a brief recall of the principles and the theoretical basis of the method implemented, called 3-omega method, which was introduced by D. Cahill are firstly given [4,5]. Then we present the results obtained during the characterization of a Si_3N_4 thin-film 470 nm thick deposited on a Si substrate (380 µm) by the 3-omega method. The latter has been widely used to measure the thermal conductivity of a wide range of materials. The process uses a thin-film metallic strip (made by an optical photolithography technique) which

serves simultaneously to thermally disturb the system and to measure the temperature variations at a remarkable point of the sample. The temperature variation in the line is then measured by detecting the third harmonic of the voltage which is proportional to the temperature variation. This voltage carries the information making it possible to extract the thermal conductivity of the material under test. In conclusion, the results obtained experimentally are compared with those resulting from an analytical solution (Cahill's solution) and those reported in the literature.

Key words: Si_3N_4 thin-film, Si substrate, thermal conductivity, 3-omega method, temperature.

Corresponding Email: a.guermoudi@univ-chlef.dz

References

[1] Andrew J. Eckel, Silicon Nitride Rocket Thrusters Test Fired Successfully [archive] http://www.grc.nasa.gov/ [archive] sur https://web.archive.org/ [archive], NASA sur la Wayback Machine, 21 avril 2000.

[2] Y. Tu and J. Tersoff, "Structure and Energetics of the Si- SiO2 Interface", Phys. Rev. Lett. Vol. 84 (19): pp. 4393, 2000. DOI:https://doi.org/10.1103/PhysRevLett.84.4393

[3] T. J. Webster, A. A. Patel, M. N. Rahaman et B. Sonny Bal, « Anti-infective and osteointegration properties of silicon nitride, poly(ether ether ketone), and titanium implants », Acta Biomaterialia, Vol. 8(12): pp. 4447-4454, 2012.

[4] D.G. Cahill," Thermal conductivity measurement from 30 to 750 K : the 3w method", Review of Scientific Instrument. Vol. 61(2): pp. 802-808, 1990.

[5] D.G. Cahill, M. Katiyar, J.R. Abelson, "Heat transport in micron thick a-Si: H films", P. R. B.; Vol. 50, pp. 6077–81, 1994.

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Magnetic and Structural Properties of FeTiO2 Nanocomposite Produced by Mechanosynthesis Technique.

Abderrahmane Younes[1], *, Rachid Amraoui[1], Asmaa Mendoud[1], Abderahim ABADA[2], Nacer Dilmi[3], and Nadia Metidji[4]

[1]Research Center in Industrial Technologies (CRTI) P.O. Box 64, Cheraga 16014 Algiers, Algeria.
[2]Laboratory of Aeronautic Science, Aeronautic Institute, University of Saad Dahlab Blida 1, Blida, Algeria
[3]Center for Development of Advanced Technologies, 20 Aout 1956, Baba Hassan, Algiers, Algeria
[4]Unité de Développement des Equipements Solaires, UDES/Centre de Développement des Energies Renouvelables, CDER Bou Ismail, 42415, W. Tipaza, Algeria
* Corresponding author: younesabdo11@gmail.com

Abstract

The synthesis of FeTiO2 nanocomposites as soft magnetic materials was achieved through the mechanical alloying technique. This study comprehensively investigates the structural, morphological, and magnetic properties of the nanocomposite at various synthesis stages using advanced characterization methods, including Scanning Electron Microscopy (SEM), Energy Dispersive Spectroscopy (EDS), X-ray Diffraction (XRD), and Vibrating Sample Magnetometer (VSM). The coercivity, magnetic remanence, and squareness ratio of Fe/TiO2 exhibited an upward trend with increasing milling time, with magnetization saturation reaching its peak values after 5 hours of milling. The FeTiO2 nanocomposite demonstrated maximum values for coercivity, magnetic remanence, and saturation magnetization, while the squareness ratio showed notable values for FeTiO2. These findings indicate that the Fe/TiO2 nanocomposite system shows significant promise as a high-frequency soft magnetic material.

Keywords: FeTiO2 nanocomposite, structural characteristics, magnetic behavior, particle morphology

P-031

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Title: Contribution to the analysis of interfacial damage of biomaterials

Liamani Samira[a]

[a]Liamani Samira' Department of machanical, University Djillali Liabes, Algeria

Abstract:

The modeling of a cracked medium is based on the result of a numerical analysis presented by the Finite Element method. Simulation and numerical analysis have developed in recent years in many fields such as biomaterial's (metal/ceramics).

This work is devoted to the analysis of residual stresses in the Ceramic-Metal junction produced in the solid state by thermo compression, as well as the variation of the stress intensity factor as a function of crack propagation. These constraints are evaluated at the interface and its close neighborhood in all directions. The intensity and distribution of these stresses depend on the physical, mechanical and thermal properties of the two jointly bonded materials. The durability of these biomaterial's and their commissioning depend on the level and distribution of these stresses and their determination is of great importance.

Key words: crack, metal, ceramics, biomaterial, MEF.

Corresponding Email: liamani2007@yahoo.fr

References

[1] F. Bouafia, B. Serier, H. Fekirini, S. Bouafia, Analyse Numériques des Contraintes Résiduelles dans les Bi-Matériaux, 3ème Conférence Internationale sur le Soudage, le CND et l'Industrie des Matériaux et Alliages (IC-WNDT-MI'12) Oran.2012

[2] S. Susan, D. Elizabeth Ceramic/metal interface structures and their relationship to atomic- and meso-scale properties, Materials Science and Engineering.2003

[3] E. Saiz, S. Foppiano, W. MoberlyChan, A.P. Tomsia, Composites Part A: Applied Science and Manufacturing.1999

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Structural, mechanical, thermodynamic and dynamic stabilities of NaCaN half-Heusler compound

Nawal Belmiloud [1]*, Fadila Belkharroubi[2], Miloud Benchehima[3], Barkahoum Larouci [4], and Mohammed Ferhat [4]

[1]Department of Engineering Physics, Faculty of Physics, Laboratory of Analysis and Application of Radiations (LAAR), University of Science and Technology of Oran Mohamed Boudiaf (USTO-MB), 1505 El Menouar 31000, Oran,Algeria.

[2]Department of Engineering Physics, Faculty of Physics, Laboratory of Physics of Materials and Fluids, University of Science and Technology USTO-MB, El Mnaouar, BP 1505, Bir El Djir 31000, Oran, Algeria

[3]Department of electronic, Faculty of electrical, University of Science and Technology USTO-MB, El Mnaouar, BP 1505, Bir El Djir 31000, Oran, Algeria.

[4]University Yahia Fares of Medea,, Algeria.

Abstract

The use of temperature opens a new direction for the design of new materials thermoelectric and development of new technology devices with a high conversion density and where the information has a very high speed. The structural, elastic, thermodynamic and dynamic properties of a cubic NaCaN half-Heusler have been investigated using the ab-initio calculation.

P-033

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Impact of Cu on the Magnetic Properties of $FeTiO_2$ Nanocomposite

Rachid Amraoui[a], Abderrahmane Younes[a], Asmaa Mendoud[a], and Abderahim ABADA[b]

[a]Research Center in Industrial Technologies (CRTI) P.O. Box 64, Cheraga 16014 Algiers, Algeria.
[b]Laboratory of Aeronautic Science, Aeronautic Institute, University of Saad Dahlab Blida 1, Blida,

Abstract:

Nanocomposite materials of $FeTiO_2$ and $FeCuTiO_2$ were synthesized via mechanical alloying. A thorough examination of their structural, morphological, and magnetic properties at various synthesis stages was performed using advanced characterization techniques, including Scanning Electron Microscopy (SEM), Energy Dispersive Spectroscopy (EDS), X-ray Diffraction (XRD), and Vibrating Sample Magnetometer (VSM). In the $FeCuTiO_2$ nanocomposite, the crystallite size reached its minimum, while the lattice strain (ε) peaked. Conversely, the $FeTiO_2$ nanocomposite exhibited maximum values for coercivity, magnetic remanence, and saturation magnetization. Interestingly, notable squareness ratios were observed for both $FeTiO_2$ and $FeCuTiO_2$. These results suggest that the Fe/TiO_2 nanocomposite system shows promise as a high-frequency soft magnetic material.

Key words: $FeTiO_2$ nanocomposite, Cu effect, structural characteristics, magnetic behavior

Corresponding Email: amrachid21@gmail.com

References

[1] X. J. Yang, W. A. N. G. Shu, H. M. Sun, X. B. Wang, and J. S. Lian, Preparation and photocatalytic performance of Cu-doped TiO_2 nanoparticles, Transactions of Nonferrous Metals Society of China **25**, 504-509 (2015)

[2] P. Akhter, A. Arshad, A. Saleem, and M. Hussain, Recent development in non-metal-doped titanium dioxide photocatalysts for different dyes degradation and the study of their strategic factors: A review, Catalysts **12,** 1331 (2022)

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Title: Phonon and electronic transport properties of FeZrTe heusler alloy for thermoelectric applications

Chewki Ougherb[a], Tarik Ouahrani[a], Naouel Boudghene Stambouli[a]

[a]École supérieure en sciences appliquées, ESSA-Tlemcen, BB 165 RP Bel Horizon, Tlemcen 13000, Algeria

Abstract:

We present a first attempt to untangle the capacity of FeZrTe half-Heusler as a thermoelectric material. The study is conducted by means of theoretical calculations based on the density functional theory (DFT) within the full-potential linearized augmented plane wave method. Phonon dispersion is computed using the finite displacement method and supercell approach by taking the equilibrium crystal structures obtained from DFT. The results show that the FeZrTe alloy is mechanically and dynamically stable in its type I structure. The FeZrTe alloy has a semiconducting character with a 1.4-eV band gap value, governed by strong p–d hybridization. The variation of thermoelectric properties as a function of carrier concentration and temperature has been studied and analyzed. All the results pave the way for the possible building of an n–p couple for a thermoelectric device.

Key words: Ab initio calculations, stability, electronic properties, thermoelectric.

Corresponding Email:

chewki_ougherb@yahoo.com

References

[1] T. Ouahrani, R. Khenata, B. Lasri, A.-H. Reshak, A. Bouhemadou, and S. Binomran, First and second harmonic generation of the XAl_2Se_4 (X= Zn, Cd, Hg) defect chalcopyrite compounds. ***Physica B: Condens. Matter*** 407, 3760 (2012).

P-035

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Title: Understanding the Mott Insulator to Superconductor Transition in Quasi-Two-Dimensional Iron-Based Compounds: A Density Functional Theory Study

Oumeria Khelladi[a], Nawel Benayad[a], Mostefa Djermouni[a], Ali Zaoui[a]

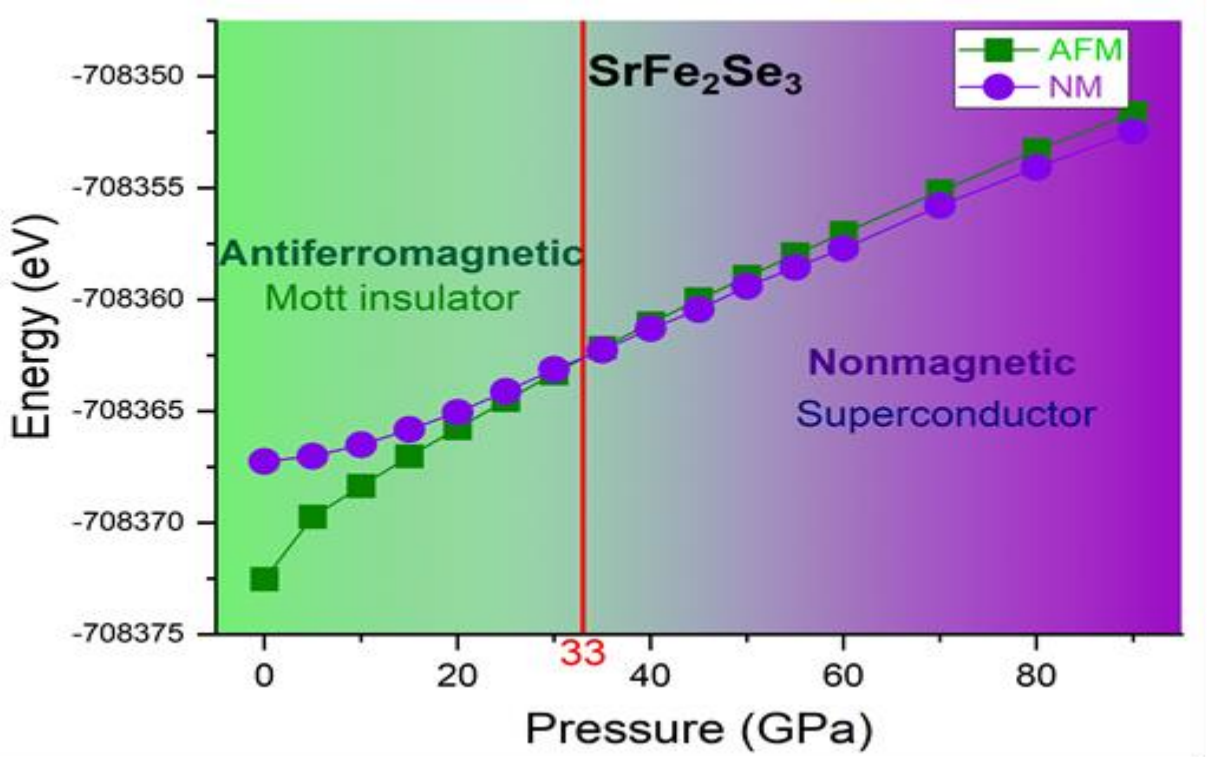
[a]Laboratoire de Physique Computationnelle des Matériaux (LPCM), Faculté des Sciences exactes, Université Djillali Liabès de Sidi Bel-Abbès , Algeria.

Abstract:

The Mott insulator to superconductor transition in iron-based compounds has attracted significant attention due to its potential for advancing fundamental understanding and enabling practical applications [1, 2]. In this study, we focus on investigating the unique behavior of quasi-two-dimensional iron-based compounds during this transition, with a specific emphasis on two-ladder iron chalcogenides [3-7].

To unravel the underlying mechanisms driving the transition, we employ Density Functional Theory (DFT) calculations. DFT has proven to be a powerful tool in exploring the electronic and structural properties of complex materials, allowing us to elucidate the intricate interplay of electronic interactions and lattice effects in these systems [8, 9].

Our investigation reveals intriguing features in the electronic structure of two-ladder iron chalcogenides AFe$_2$$Ch_2$ (A= Ca, Sr, Ba; and Ch= chalcogenides S and Se) that give rise to the Mott insulating state. The geometric arrangement of the compound and its inherent anisotropic nature play a crucial role in shaping its electronic properties and facilitating the transition to a superconducting state. Furthermore, we analyze the effect of pressure, on the Mott insulator to superconductor transition in these compounds.



The findings from our DFT-based study shed light on the underlying physics governing the intriguing behavior of quasi-two-dimensional iron-based compounds during the transition. Additionally, our results provide valuable insights into the potential design principles for new materials with tailored properties for superconducting applications. These outcomes contribute to the broader understanding of high-temperature superconductivity and pave the way for future experimental investigations and technological advancements in this field.

Key words: The Mott insulator, Superconductor transition, Iron-based compounds, DFT.

Corresponding Email:khelladioumeria@gmail.com

References

[1] Q. Si and E. Abrahams, Phys. Rev. Lett. **101**, 076401 (2008).

[2] M. R. Norman, Physics **1**, 21 (2008).

[3] T. Yamauchi, Y. Hirata, Y. Ueda, and K. Ohgushi, Phys. Rev. Lett. **115**, 246402 (2015).

[4] H. Takahashi, A. Sugimoto, Y. Nambu, T. Yamauchi, Y. Hirata, T. Kawakami, M. Avdeev, K. Matsubayashi, F. Du, C. Kawashima, H. Soeda, S. Nakano, Y. Uwatoko, Y. Ueda, T. J. Sato, and K. Ohgushi, Nat. Mater. **14**, 1008 (2015).

[5] J. Ying, H. Lei, C. Petrovic, Y. Xiao, and V. V. Struzhkin, Phys. Rev. B **95**, 241109(R) (2017).

[6] J. M. Caron, J. R. Neilson, D. C. Miller, A. Llobet, and T. M. McQueen, Phys. Rev. B **84**, 180409(R) (2011).

[7] H. Y. Hong and H. Steinfink, J. Solid State Chem. **5**, 93 (1972).

[8] Y. Zhang, L. F. Lin, J. J. Zhang, E. Dagotto, and S. Dong, Phys. Rev. B **95**, 115154 (2017).

[9] Y. Zhang, L.-F. Lin, J.-J. Zhang, E. Dagotto, and S. Dong, Phys. Rev. B **97**, 045119 (2018).

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Structural, mechanical, thermodynamic and dynamic stabilities of NaCaN half-Heusler compound

Lamia Drici[a], Fadila Belkharroubi[a,b] ,Ibrahim Ameri[a], Blaha lamia Farah[a], Mohammed Ameri[a].

a Laboratory of Physical Chemistry of Advanced Materials (LPCMA), University of Djillali Liabes, BP 89, Sidi Bel-Abbes, 22000, Algeria. a,b Genius Physics Department, Faculty of Physics, University of Sciences and Technology USTO-MB, 31000, Oran, Algeria

Abstract

Our comparative study is carried out on different structural, elastic, electronic, and optical properties of two new half-Heusler CaCuP and CaAgP compounds by using first-principles calculations based on density functional density. The generalized gradient approximation (GGA) is used for studying exchange and correlation effects. The mBJ-GGA approximation is also employed to give a better approximation of the energy bandgap for the two CaCuP and CaAgP compounds. Our two compounds are more stable in cubic structure type I structure and the lattices parameters obtained in good agreement with other available data. The two compounds are mechanically stable; the calculated elastic constants strictly obey the stability criteria with brittle behavior, isotropic, and ionic nature in cubic structure type I. The electronic properties have pointed to a semiconductor behavior for the two compounds and have shown a direct gap Γ→Γ equal to 1.785 eV for CaCuP and 1.621 eV for CaAgP with mBJ-GGA approximation. The study of optical properties with mBJ-GGA approximation as a function of photons energy for a wide range between 0 and 27 eV reveals that the two half-Heusler CaCuP and CaAgP compounds display the maximum reflectivity and absorption in the ultra violet range. Keywords: DFT . CaCuP and CaAgP . Semiconductor . Ultra-violet

P-037

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Title: Study of the physical properties of halogen-based perovskite materials

MerahSomia[a], Sahnoun Omar[a], Riane Howaria[a]

[a] Department of physics/Research Institute LPQ3M University of Mascara, Algeria

Abstract:

Optoelectronic properties and high power conversion efficiency make lead halide perovskites an ideal material for solar cell applications. However, the toxic nature of lead and the instability of organic cations limit their use and commercialization. Suggesting an alternative, we present our DFT-based first principles calculations of Cs2PbX6 (X = Cl, Br, and I) using the highly acclaimed modified Becke Johnson (mBJ) and. We report on a strong optical absorption in the visible region with a small effective mass and direct band gap of 2.03, 1.95, and 1.516 eV for Cs2PbCl6, Cs2PdBr6, and Cs2PbI6, respectively. Our results suggest that our compounds are suitable for applications as light absorption layers in perovskite solar cells. Also, based on their optical properties, we concluded that our studied perovskites are classified as materials in the visible range.

Key words: Ab-initio, first-principles,DFT ,

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

On Vortices structures in non ideal magnetized dusty plasma

El Amine Nebbat

Faculty of Sciences, University of Algiers (1), and Laboratory of (LSDME), University of Algiers (1), Algiers 16000, Algeria. E. mail : e.nebbat@univ-alger.dz

Abstract

Dusty plasma usually contain small dust particles (nano to micron-sized) which are charged and embedded in a partially ionized plasma of electrons, ions, and neutral gas particles. These plasmas may be encountered in a wide range of situations spanning astrophysical to industrial situations. Several technological applications have stimulated the development of plasma physics, e.g. radiocommunications, surface treatments by plasma in micro-electronics (engraving and deposition of thin films), gas lasers, cutting of metals by plasma torch, etc. In laboratory, the grain (dust) rearrange themselves collectively give rise to numerous nonlinear solution such as vortices. The vortices are formed under certain conditions when a rotational motion around a core, is triggered. These non-linear structures that have been observed in many laboratories are investigated by way of various theoretical models to explain their characteristics. Nebbat and Annou proposed a time dependent non-linear model that considers vortices as a consequence of an instability, and where the plasma is considered ideal [1]. In this work the azimuthal velocity of the vortex was studied, the results are in perfect agreement with the experimental work. However, from thermodynamics point of view, the system is open as plasma particles are gained and lost due to attachment by dust grains, therefore, the ideal gas approximation ceases to be valid. The nonideal effects are introduced throught a van der waals equation. In this work, as the plasma departs form ideality, a Van Der Waals equation of state of the plasma is privileged where numerous potentials are introduced. The model by Nebbat and Annou is augmented and the results are compared to those found in Ref.[1].

Keywords : plasma, dust, velocity, ideal, non ideal

P-039

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Planning the Trajectory of a Mobile Robot Using the A(*) Star Algorithm

N. BOUAM[a], A. MESSEI[b]

[a]Department of Electrical Engineering, Faculty of Technology, Yahia Fares Medea University, Medea, Algeria
[b]Research Nuclear Centre of Birine, Ain-Oussera, Algeria

Abstract:

In many industrial fields, mobile robots are widely used these days. Research on the mobile robot's path planning is one of the most important aspects of improvements on the mobile robot field. A mobile robot's path planning involves finding a collision-free trajectory, through the robot's environment with obstacles, from a specified starting location to a desired destination while meeting certain optimization criteria. In the path planning of mobile robot moving from its own position to the target point, the traditional A-star (A*) algorithm is widely used as the most popular path planning algorithm in robots. However, there are many redundant inflection points in the path planned by the traditional algorithm, and the path length is long. The large peak path at the inflection point is not smooth enough, which leads to the problem of path safety. To solve the above problems, an A-star algorithm is proposed and used. The objective of this work consists in the development of a computer program on Matlab software, which allows the determination of the navigation optimal trajectory in a two-dimensional environment at minimal time. The method is based on the A(*) star algorithm, which is widely used in practice according to its advantages and the results obtained, compared to other algorithms. The simulation results obtained are in good agreement with those of the literature and show the ability of this algorithm to solve the given problem.

P-040

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Title: Influence of Ag doping on opto-electrical properties of copper oxide thin layer deposited by spray pyrolysis root

Nardjes Randa HAMDAOUI[a], Younes MOUCHAAL[b] , Lamia BARKAT[a] and Abdelbacet KHELIL[a]

[a] Laboratoire De Physique des Couches Minces et Matériaux pour L'Electronique (LPCMME), Faculté des Sciences Exactes et Appliquées, Université Oran 1, Oran, Algeria
[b] Département de Physique, Faculté des Sciences Exactes, Université Mustapha Stambouli , Mascara, Algeria.

Abstract:

Ag doped copper oxide thin films were grown on glass substrate by spray-Pyrolysis method in order to study the influence of the Ag doping rate in the optical, electrical and morphological properties of these thin layers.

The synthesized copper oxide thin films were doped with (1%-2%-4% and 8%) of Ag and annealed at 400°C for 2h, then have been characterized via optical, electrical and morphological techniques.

Optical Transmission of prepared samples were measured by UV-vis spectroscopy, these measurements showed that the doping rate had strong effect on the optical properties and it indicated that the transparency is reduced with increased silver content [1].

UV-vis spectroscopy measurement also showed that the band gap value of the prepared copper oxide thin films is varied between 1.30eV and 1.39eV by varying the doping rate.

Electrical properties of samples were measured by four point probe instrument; the analysis showed that variation in doping rate at 1% had a remarkable effect on electrical properties; it indicated the maximal conductivity of 15.4.103 $(\Omega .m)^{-1}$.

Morphological properties were estimated using atomic force microscopy (AFM); the analysis showed that with the increase in Ag content, the surface roughness is found to decrease [2].

These results confirm that the spray pyrolysis deposition method of copper oxide thin layers with adequate Ag doping rate can be applied to produce suitable transparent and conductive structures towards optoelectronic applications.

Key words: Copper oxide, Spray pyrolysis, Ag Doping , Uv-Vis Spectroscopy, Hall Effect, AFM.

Corresponding Email: nardjes.randa@gmail.com

References

[1] S. Das et T. L. Alford, « Structural and optical properties of Ag-doped copper oxide thin films on polyethylene napthalate substrate prepared by low temperature microwave annealing », Journal of Applied Physics, vol. 113, n° 24, p. 244905, juin 2013, doi: 10.1063/1.4812584.

[2] D. Berra, S. E. Laouini, B. Benhaoua, M. R. Ouahrani, D. Berrani, et A. Rahal, « Green synthesis of copper oxide nanoparticles by pheonix dactylifera l leaves extract ».

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Predictive Modeling of Intrinsic Viscosities in Polymer Solutions Using Advanced Algorithms

Mohamed KouiderAmar *[1] Mohamed Hentabli[1]

[1]Laboratory of Biomaterials and Transport Phenomena (LBMPT), Faculty of Technology, University YahiaFares of Médéa26 000, Médéa, Algeria. Email: kouideramar.mohamed@univ-medea.dz

Abstract

This research aims to improve predictive modeling in polymer solutions using artificial intelligence techniques. It proposes a novel approach for predicting intrinsic viscosities of polymer solution mixtures using moleculardescriptors for solvents and polymer monomers. The Artificial Neural Network-Antlion Optimizer (ANN-ALO) surpasses the linearmodel (MLR)andSVR RBF-ALO, exhibiting exceptional predictiveperformance.Optimized hyperparameters lead toaR2 of 0.7487 during testing, with the model'sgeneralizabilityconfirmed on the entire dataset (R2 = 0.7872).Themodel demonstrates itsaccuracy,offeringarobustand generalizable solution for predicting transformed intrinsic viscosityinpolymersolutions.

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Structural and photoluminescence properties of Li co- doped $(Gd_xLu_{1-x})_2O_3$: 5% Eu^{3+} nanomaterials scintillators prepared by sol gel method

F.Riahi[a], L.Guerbous[b], W.Zerman[c], C.Djebari[d]

[a]*Nuclear Research Centre of Birine, Bp 180 - Ain Oussera-17200 - Djelfa- Algeria*
[b]*Nuclear Research Centre of Algiers , 02, Boulevard Frantz Fanon, B.P. 399, Algiers (16000), Algeria*
[c]*Faculty of sciences, Saad Dahleb Blida1 University, Blida(9000),Algeria*
[3]*Faculty of sciences,* August, 20th; 1955 University of Skikda, Algeria;

Abstract:

The Gd_2O_3, Lu_2O_3, $(Lu_{0.5}\ Gd_{0.5})_2O_3$, nanomaterials doped Europium trivalent Eu^{3+} and co-doped Li have been elaborated by the sol-gel route, using gadolinium, Lutetium and europium nitrates as precursors. The structure and luminescence properties of the as-prepared products were characterized by X-ray diffraction (XRD) and photoluminescence spectroscopy. The results obtained by means of X-ray diffraction, confirmed the presence of the cubic structure with space group $Ia\bar{3}$ of all powders, The fluorescence spectrum shows that the powders generate a characteristic red emission when stimulated by ultraviolet light with a wavelength of 250 nm, which corresponds to the $^5D_0$–^7F_J (J = 0, 1, 2 and 3) transitions of trivalent europium ion, with the most intense red emission at 611nm.

In this contribution, the influence of Lithium on particle size and luminescence properties was investigated. The results show that excess of the concentration of co-dopant Li^+ ion, presented greater particle size and higher luminescence intensity

Key words: nanomaterial, sol-gel, photoluminescence, luminescence

Corresponding Email:
F.riahi@crnb.dz

P-043

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Title: Elaboration et caractérisation de composites à matrice polyurethane nanochargée avec des nanoparticules de ZnO-La

Malika Saidi[a], Zakia Chelli[a], Saliha Rabehi[a], Rachida Douani [a], Nouara lamrani[a,] Ahcéne Chaouchi [a], Yannick Lorgoilloux [b], Mohamed Rguiti [b], Christian Courtoisb

[a] Department de Chimie, Laboratoire de Chimie Appliquée et Génie Chimique de l'Université Mouloud Mammeri de Tizi-Ouzou,
[b] Univ. Polytechnique Hauts-de-France, F-59313 Valenciennes, France

Abstract:

Ce travail est focalisé sur l'élaboration de composites à matrice polyurethane(PU) renforcées par des nanoparticules d'oxyde de zinc dopées avec du Lanthan à différentes proportions massiques.

Dans un premier temps, nous avons preparé la poudre ZnO-La par une méthode chimique qui est la voie sol gel, puis nous avons élaborés des composites.

Les matériaux élaborés ont été caractérisés par différntes techniques d'analyses (MEB, infra rouge) et par impédencemétrie (propriétés diélectriques et électriques)

Les observations par microscopie électronique à balayage des films composites ont montré une distribution des particules de façon uniforme et homogène dans la matrice PU. La caractérisation par spectroscopie infrarouge a montré que les différents échantillons contiennent la bande caractéristique de ZnO-dopé, cette dernière diminue en intensité avec la décroissance de la quantité de charges incorporées dans le composite. La caractérisation par spectroscopie d'impédance des films composites a montré que : L'introduction des particules de ZnO-La dans la résine polyuréthane engendre une amélioration des caractéristiques diélectriques du composite ainsi qu'une augmentation de La conductivité avec la fréquence,

ce qui peut être expliquée par la réduction de la polarisation de charges d'espaceLes résultats obtenus ont montré que le composite à 15% ZnO-La présente les meilleures propriétés.

Key words: Composite, polymére, diélectrique, électrique, l'oxyde de zin

Corresponding Email:
malika.saidi@ummto.dz

References

[1] .....
[2] .....

P-044

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Elaboration de détecteurs d'humidité à base de biocomposites kératine/ x% nanoparticules d'argent.

R. DOUANI, H. HAMMOUHE, M. SAIDI, M. OUGHANEM, A. CHAOUCHI.

Laboratoire de Chimie Appliquée et Génie Chimique, Université Mouloud MAMMERI de Tizi Ouzou, Algérie.

Abstract:

L'objectif mené au cours de ce travail, est la caractérisation électriques et diélectriques de couches minces à base de biocomposites kératine/x%Ag et leur application comme capteur d'humidité. La kératine a été extraite à partir de laine du mouton par la méthode d'hydrolyse alcaline et les nanoparticules d'Argent ont été synthétisées en utilisant l'extrait du romarin par le procédé de la synthèse verte. Les capteurs ont été testé dans une plage d'humidité relative allant de 15 à 94% sous une fréquence de 100 Hz.

Les résultats ont montré une sensibilité à la présence des molécules de vapeur d'eau, qui s'est traduit par l'augmentation de la valeur de la capacité (Cp) en fonction du taux d'humidité relative. Les capteurs à base du biocomposite ont montré une sensibilité précoce à la présence des molécules de vapeur d'eau comparant au capteur à base de la kératine pure. Un nette réduction de la valeur de l'hystérésis a été également enregistrée avec l'augmentation du pourcentage de nanoparticules d'Ag dans la matrice kératinique. Les tracés de la variation de la sensibilité des couches sensibles en fonction du taux d'humidité (RH%), ont montrés que l'ajout des nanoparticules d'Argent améliore les propriétés de détection de l'humidité de la kératine.

Key words: kératine, nanoparticules d'Argent, biocomposite, capteurs d'humidité.

Corresponding Email:

Rachida.douani@ummto.dz_____

References

P-045

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Optimisation of a heterojunction solar cell: InGaN/SnS

H. Mazari[a], K. Ameur[a], A. Boumesjed[a], N. Benyahya[a], N. Benseddik[a], Z. Benamara[a]

[a] Applied Microelectronics Laboratory, Department of Electronics, Faculty of Electrical Engineering, Djillali Liabès University of Sidi Bel Abbes, BP: 89, 22000, Sidi Bel Abbes, Algeria

Abstract:

Photovoltaic electricity production is expected to be one of the key technologies for achieving a low-carbon society in the future. Among photovoltaic solar technologies, the heterojunction stands out for its high conversion efficiencies of light energy into electricity. Its use, which is based on the concept of broadening spectral conversion, leads to a better exploitation of the solar spectrum by widening the useful range of the spectrum. Gallium indium nitride (InGaN) and tin sulfide (SnS) emerge as the fundamental materials used in photovoltaic technology and in the manufacture of InGaN/SnS heterojunction photovoltaic cells using SnS as the absorber material [1]. In our work, we relied on the most suitable software for photovoltaic conversion of semiconductor devices, the SCAPS-1D simulation software [2]. This is done through numerical simulation of the current-voltage (I-V) characteristic under AM1.5G solar illumination conditions. The results obtained showed that the $In_{0.2}Ga_{0.8}N$/SnS heterojunction solar cell could achieve an efficiency exceeding 30%. The spectral response extends well from visible to infrared (946 nm).

Key words: solar cell; heterojunction; . InGaN; SnS; efficiency.

Corresponding Email: hmazari2010@gmail.com

References

[1] A. Mishra, « Photovoltaic properties of SnS based solar cells », International Journal of Mechanical And Production Engineering, Volume- 2, Issue- 3, 45-46, **2014**.

[2] M. Burgelman, J. Verschraegen, S. Degrave, P. Nollet, "Modeling Thin- film PV Devices",Progress in Photovoltaics: Research and Applications, Vol. 12, pp.143-153, **2004.**

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Analysis of radioactive materials behavior in the environment during the nuclear accident

A. Dadda Khorsi*[a], A. L. Cheridi Deghal[a], A. Bouam[b], A. Dahia[b], B. Bouali[c]

[a]Nuclear Safety and Radiation Protection Division, Nuclear Research Centre of Birine, P.O. box 180 Ain-Oussera Algeria
[b]Nuclear Technology Division, Nuclear Research Centre of Birine, P.O. box 180 Ain-Oussera, Algeria
[c]Process Engineering Laboratory, Ammar Telidji University, Laghouat, 03000, Algeria

Abstract:

On April 26, 1986, an accident occurred at the fourth unit of the Chernobyl nuclear power plant [1], which, according to its scale and consequences, became the largest accident in the history of nuclear power. The accident caused the release of a large number of radio nuclides, which determined the radio nuclide contamination of Ukraine, Belarus, Russia, and other states, as well as the radiation dose of the population in these territories. The physico-chemical forms of radioactive material (radio nuclides) in the Chernobyl release have a significant impact on their environmental behavior, bioavailability, solubility, health effects and ecological [2]. After the accident, some radionuclides were released during the oxidation and diffusion of the nuclear fuel. After reaching the atmosphere, the more volatile radioactive substances remained in the gas phase, while the less volatile aggregated on construction material and atmospheric aerosol particles.

Using two codes Origen [3] and HOTSPOT [4], in this work, we have analyzed the concentration of Iodine and Cesium isotopes and their radiological effects during the first stage of the accident on the environment and humans.

The results of atmospheric transport and deposition of radioactive material on the surface show very high contamination. It can be concluded that in cases of a major radiation accident,

the potential for risks to the public and the environment increases due to the release of radioactive materials in the air [5].

Key words: Radioactive material, environment, Radiological contamination, Simulation, codes.

Corresponding Email: daddaamel@hotmail.com, a.dadda@crnb.dz

References

[1] IAEA (International Atomic Energy Agency) (1986) Summary report on the post-accident review meeting on the Chernobyl accident, safety series no. 75-INSAG-1. IAEA, Vienna

[2] Salbu B, Krekling T, Oughton DH (1998) Characterization of radioactive particles in the environment. Analyst 123:843 – 849

[3] Koyama, Kinji, Naoki, Yamano, shun-ich, Miyasaka, 1979. ORIGEN-JR: A Computer Code for Calculating Radiation Sources and Analyzing Nuclide Transmutations. Japan Atomic Energy Research Institute JAERI-M-8229.

[4] Steven, G., 2020. Homann and fernande aluzzi, HotSpot health physics codes, version 3.1.2. In: National Atmospheric Release Advisory Center. Lawrence Livermore National Laboratory, Livermore, CA 94550, USA.

[5] IAEA, 2020. Case Study on Assessment of Radiological Environmental Impact from Potential Exposure. IAEA-TECDOC-1914, VIENNA.

P-047

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Numerical study of the ambient temperature influence on a vortex tower performance

Deghal Cheridi A. L.[*a], Bouam.A[b], Dadda.A[a], Dahia.A[b], Hadjam.A[b]

[a]Nuclear Safety and Radiation Protection Division, Nuclear Research Centre of Birine, B.P 180 Ain-Oussera, Algeria.
[b]Nuclear Technology Division, Nuclear Research Centre of Birine, B.P 180 Ain-Oussera, Algeria.

Abstract:

The growing consumption of traditional sources of energy as the population grows has resulted in their depletion and an increase in environmental pollution [1]. Therefore the search for new sources of energy at the same time that do not pollute the environment has become essential. Indeed, several researches have been interested to present new efficient renewable energy systems. One of these systems is the Atmospheric Vortex Engine (AVE) [2]. Is one of the most promising systems for providing electrical energy to humanity and preserving the environment.

The purpose of this study is to model and simulate the ability of a novel vortex tower to generate airflow using the Relap5 code. Furthermore, a parametric study is presented to determine the effect of ambient temperature on tower performance in order to achieve operating conditions. The goal of this device is to generate more electrical energy by reusing lost energy that has previously been transferred to the environment to cool an installation. As a result, the primary information sought here is the best location in the air path where the velocity would be favorable for turbine installation. The vortex tower model was developed and validated using numerical and experimental results, and it was well accepted. According to the simulation results, this vortex tower's configuration can produce an air flow with a maximum velocity of 5.5411m/s at 0.560 m from the base. As a result, a turbine can be

installed in this location to maximize kinetic energy. Furthermore, the simulation demonstrated the influence of the ambient temperature on the performance of this device. Revealing that the upward airflow is inversely proportional to the ambient temperature.

Key words: Vortex tower, Artificial vortex generation, Ascendant air flow, Modeling and simulation, Relap5, Ambient temperature

Corresponding Email: al_cheridi@yahoo.fr, a-l.deghal@crnb.dz

References

[1] BP, Statistical Review of World Energy, 2021, pp. 8–21.

[2] A.T. Mustafa, H.H. Al-Kayiem, S.I.U. Gilani, A review of the vortex engine, WIT Trans. Ecol. Environ. 2 (2013), 911–920.

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Theoretical Prediction of Monolayer $ScHfNO_2$ as a Potential Material for Ultraviolet Photodetection

Mounir Ould-Mohamed [a], Tarik Ouahrani [b]

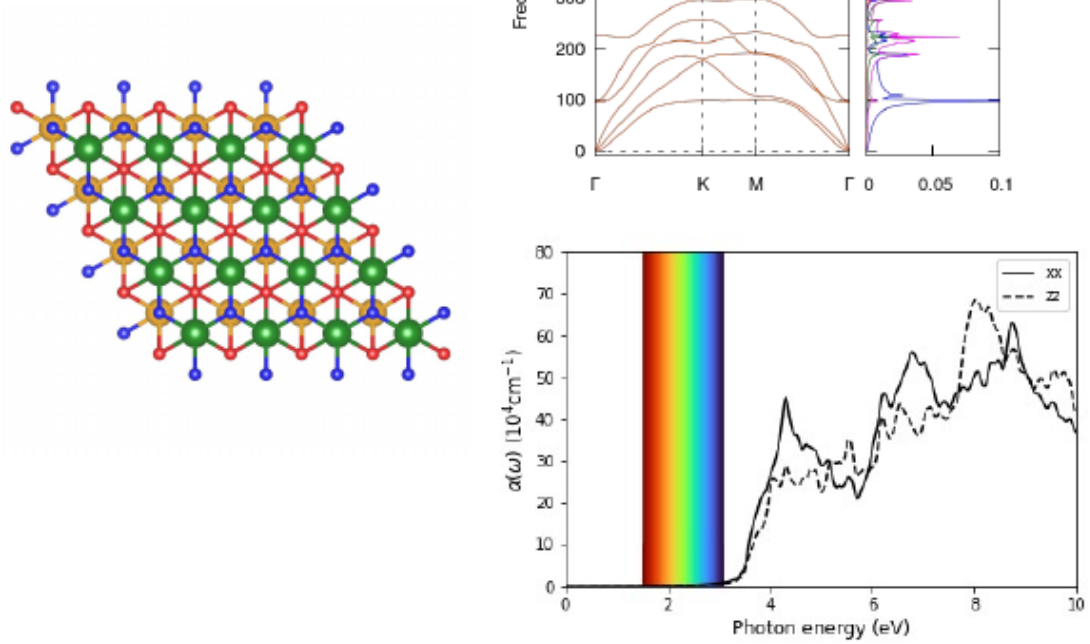
[a]LPTHIRM, Département de physique, Faculté des sciences, Université Saâd DAHLAB- Blida 1, B.P. 270 Route de Soumâa, 09000 Blida, Algeria

[b]Laboratoire de Physique Théorique, Université de Tlemcen, BP 119, 13000, Algeria

Abstract:

Over the past few years, two-dimensional (2D) materials have garnered significant research attention due to their remarkable electronic, mechanical, electromechanical, thermoelectric, photocatalytic, and optoelectronic properties. In this work, we explore the structural and optical properties of a novel two-dimensional $ScHfNO_2$ monolayer by means of ab initio calculations. The stability of the $ScHfNO_2$ monolayer, including its dynamic, thermal, and mechanical stability, was confirmed through phonon dispersion curves, AIMD calculations, and elatsic constant calcuations , respectively. It was found that the monolayer $ScHfNO_2$ exhibits a indirect bandgap of 3.089 eV according to the Pbesol functional (4.461 eV according to Heyd–Scuseria–Ernzerhof (HSE06) hybrid functional). The considerable absorption in the UV region of the $ScHfNO_2$ monolayer makes it a potential candidate material for optoelectronic applications such as UV-detectors.

Key words: ab initio calculations, $ScHfNO_2$ monolayer , Phonon dispersion calculations UV-detectors



Corresponding Email: ouldmohamed_mounir@univ-blida.dz

References

[1] Giannozzi, Paolo, Oliviero Andreussi, Thomas Brumme, Oana Bunau, M. Buongiorno Nardelli, Matteo Calandra, Roberto Car et al. "Advanced capabilities for materials modelling with Quantum ESPRESSO." *Journal of physics: Condensed matter* **29**, no. 46 2017 : 465901.

[2] T. Ouahrani and R. M. Boufatah, Understanding the Semiconducting-to-Metallic Transition in the CF_2Si Monolayer under Shear Tensile Strain, *Crystals*, 2022, **12**, 1476

P-049

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Multi-Objective Optimization of Biodegradable Polymer-Based Microspheres Loaded with Candesartan Cilexetil

Ahmed Chabane [a,c]*, Mohamed Kouider Amar[b,c], Mohamed Hentabli[b,c], Fatiha Bouchal[a], Farouk Rezgui[a]

[a]Organic Materials Laboratory, Department of Engineering Processes, Faculty of Technology, Université de Bejaia, Bejaia, Algeria
[b]Laboratory of Biomaterials and Transport Phenomena (LBMPT), Faculty of Technology, University Yahia Fares of Médéa 26 000, Médéa, Algeria.
[c]Laboratory of Quality Control, Development Department, SAIDAL of Medea, 26000, Médéa, Algeria.

Abstract:

Multi-objective optimization (MOO) techniques are crucial in addressing complex engineering problems with conflicting objectives, particularly in pharmaceutical applications where optimizing drug delivery systems requires balancing encapsulation efficiency and drug release properties. This study focuses on optimizing a biodegradable micro-polymeric carrier system for drug delivery, specifically targeting the encapsulation efficiency and drug release of candesartan cilexetil antihypertensive drug. Using response surface models to formulate the problem definition, five prominent MOO algorithms were employed: RNSGA-III, MOEAD, RVEA, C-TAEA, and AGE-MOEA. The optimization process aimed to generate Pareto fronts representing compromise solutions between encapsulation efficiency and drug release. Results revealed inherent conflicts between objectives, with improvements in encapsulation efficiency often leading to a decrease in drug release rate. The Pareto fronts demonstrated non-linear relationships between the objectives, showcasing the trade-offs between them. Evaluation of MOO algorithms using performance metrics such as hypervolume, generational distance, inverted generational distance, spacing, maximum spread, and spread metric

provided insights into their strengths and weaknesses. Among the evaluated algorithms, RNSGA-III emerged as the top performer, achieving a Weighted Sum Method (WSM) score of 82.0776, followed closely by MOEAD with a WSM score of 80.8869. RVEA, C-TAEA, and AGE-MOEA also demonstrated competitive formulation quality, albeit with slightly lower WSM scores. In conclusion, the study underscores the importance of MOO techniques in optimizing pharmaceutical formulations, providing valuable insights for decision-makers in selecting optimal formulations that balance conflicting objectives effectively.

Key words: Multi-objective optimization, Polymeric Microspheres, Pareto front, Encapsulation efficiency, Drug release.

*Corresponding Email: ahmed.chabane@univ-bejaia.dz

References

[1] Pereira, J.L.J., Oliver, G.A., Francisco, M.B., Cunha, S.S., and Gomes, G.F. (2022) A Review of Multi-objective Optimization: Methods and Algorithms in Mechanical Engineering Problems. Arch. Comput. Methods Eng. 29, 2285–2308

[2] Sharma, S. and Kumar, V. (2022) A Comprehensive Review on Multi-objective Optimization Techniques: Past, Present and Future. Arch. Comput. Methods Eng. 29, 5605–5633

[3] Kouider Amar, M., Rahal, S., Laidi, M., Boukessani, H., Hallouane, H., Kerbouci, K., and Zemirline, H. (2023) A comparative study of multi-objective methods and algorithms for optimizing emulgels consistency and drug diffusion. J. Drug Deliv. Sci. Technol. 89, 104996

[4] Kouider Amar, M., Rahal, S., Laidi, M., Kouar, I., Bourahla, R.F.E.-K., Akouche, Y., and Bouaraba, R. (2024) Balancing competing objectives in bigel formulations using many-objective optimization algorithms and different decision-making methods. Eur. J. Pharm. Biopharm. 195, 114167

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

The amplitude distribution of the total enthalpy flux at the cathode interface in TIG welding

Merazi Sayah[1] , Leila Belgacem[1]

[1]Research Center in Industrial Technologies – CRTI – Algiers, Algeria 1
s.merazi@crti.dz, ll.belgacem@crti.dz

Abstract

Understanding the amplitude distribution of total enthalpy flux at the cathode interface in Tungsten Inert Gas (TIG) welding is vital for comprehending heat transfer dynamics and ensuring optimal weld quality. This study focuses on analyzing schemes of enthalpy flux distribution, incorporating both thermal and kinetic energy components, at the cathodic interface during TIG welding processes. Utilizing COMSOL numerical simulations to simulate cathode/arc coupling, various factors influencing amplitude distribution such as welding parameters, electrode geometry, and material properties are examined. The findings underscore the necessity of regulating amplitude distribution to achieve desired welding outcomes, including enhanced penetration depth, minimized heat-affected areas, and improved weld strength. This research contributes to refining TIG welding processes and advancing understanding of thermal phenomena at the cathodic interface.

Keywords –cathode interface, enthalpy flux, amplitude distribution, heat transfer dynamics, TIG welding, welding parameters, computational simulations.

P-051

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Predictive Study and Simulation of the Photoelectric Behavior of a $CH_3NH_3PbI_3$ Perovskite Solar Cell

Kheira Ameur [a], Nadia Benseddik [b], Halima Mazari [a], Kheira Ouari [c], Mohammed Chellali [a], Zineb Benamara [a]

[a] Department of Electronics, University Djillali Liabes of Sidi Bel Abbes, Applied Microelectronics Laboratory, 22000 Sidi Bel Abbes, Algeria
[b] Department of Physics, University Djillali Liabes of Sidi Bel Abbes, Condensed Matter and Sustainable Development Laboratory, 22000 Sidi Bel Abbes, Algeria
[c] Department of Automatics, Applied Materials Laboratory, Research Center (CFTE), University Djillali Liabes of Sidi Bel Abbes, 22000 Sidi Bel Abbes, Algeria

Abstract:

The performance of a solar cell can be enhanced through the optimization of technological parameters such as thickness and doping, ensuring high values for both short-circuit current, conversion efficiency, open-circuit voltage, and fill factor.
In this paper, we relied on the SCAPS software to optimize these technological parameters for $CH_3NH_3PbI_3$ perovskite solar cell [1] with an N-I-P junction under AM1.5G solar irradiance conditions. Subsequently, the determined values were employed to simulate the current-voltage (J-V) characteristic and the spectral response curve. Furthermore, we investigated the effect of the metal work function (anode/HTL contact) on the photovoltaic parameters of the solar cell.

Key words: Solar cell, Photovoltaic Parameters, Perovskite $CH_3NH_3PbI_3$, Simulation,

Corresponding Email:

Kheira_ameur@yahoo.fr

References

[1] Iori Ono, Takeo Oku, Atsushi Suzuki, Yugo Asakawa, Shuhei Terada, Masanobu Okita, Sakiko Fukunishi, and Tomoharu Tachikawa, "Fabrication and characterization of $CH_3NH_3PbI_3$ solar cells with added guanidinium and inserted with decaphenylpentasilane'', Japanese Journal of Applied Physics 61, SB1024 (2022).

P-052

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Effect of Shielding Gas on Tungsten Cathode Performance during DC TIG Welding

Belgacem leila[1], Merazi Sayah[1], Kaddour Houria[2], Benharat Samira[1], Sakmeche Mounir[3]

[1]Research Centre in Industrial technologies – CRTI- Cheraga-Algiers - Algeria

[2] University of Science and Technology Houari Boumediene , Bab Ezzouar, Algeria

[3]Laboratory of Catalytic Materials and Industrial Processes (LMPCI), Department of hydrocarbons and renewable energies, Faculty of Science and Technology. University of Adrar, National High way No. 06. Adrar 01000, Algeria

Abstract- A comparative study was conducted on the effect using Helium and Argon on the operational performance of tungsten electrodes. The main objective is to investigate how the nature of gas influences the temperature distribution and current density at the cathodic tip when assembling AISI 4340 steel plates by DC TIG welding. Data collected through the Comsol software, combining physical phenomena of cathode / plasma, indicate that the use of helium leads to a significant increase in temperature at the cathodic tip, resulting in noticeable deterioration compared to argon. Furthermore, although the current density distribution is similar for both gases studied, the measured values are substantially higher with helium.

Keywords: Shielding gas, TIG welding process, Current density, temperature distribution, Cathode tip

Reference

[1] Liu ZM, Fang YX, Chen SY, et al , « Focusing cathode tip characteristics in cooling tungsten ». Energy 167:982–993, 2019

[2] Nahed C, Gounand S, Medale M (2022) A numerical study of the effects of cathode geometry on tungsten inert gas type electric arcs. Int J Heat Mass Transf 182:121923, 2022

P-053

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Title: Adsorption and degradation of methylene blue (MB) Dye Using nonlinear optical (NLO) active copolymer composite.

Presenting author's Arbouz Imene [a], Chadli Redouane [b], Guemra Kaddour [c]

[1] Arbouz Imene' Laboratory of Physical and Macromolecular Organic Chemistry, Department of Chemistry, Faculty of Exact Sciences, "Djillali Liabes"BP 89 University of Sidi Bel Abbes Algeria
[2] Chadli Redouane' Laboratory of Physical and Macromolecular Organic Chemistry, Department of Chemistry, Faculty of Exact Sciences, "Djillali Liabes"BP 89 University of Sidi Bel Abbes Algeria
[3] Guemra Kaddour3 Laboratory of Physical and Macromolecular Organic Chemistry, Department of Chemistry, Faculty of Exact Sciences, "Djillali Liabes"BP 89 University of Sidi Bel Abbes Algeria

Abstract:

Our study entails two parts: The first reports on the synthesis of a novel 4,4'-[benzene-1,4-diyldi(E)diazene-2,1-diyl]-Di benzaldehyde monomer which was achieved by an electrophilic substitution of the para-bis-diazonium anion on two Benzaldehyde equivalents in an alkaline medium, the para-bis-diazonium anion is carried out by the reaction of potassium nitrate on para-phenylene-diamine in an acidic medium. Then we carried out a copolymerization of this new monomer with Para phenylene diamine in the presence of activated clay Mg-H+, the new monomer and the copolymer obtained are analyzed by 1H and 13C nuclear magnetic resonance (NMR), and infrared (IR) spectroscopy, and also analyzed by ultraviolet–visible (UV–vis) spectroscopy in order to determinate the gap energy. The experimental optical gap energy was obtained using the Tauc method. Based on our results, we have concluded that the synthesized copolymer is a good candidate for the design of organic NLO materials.

Then from our synthesized copolymer and the activated clay Mg_H+ (Maghnia clay),

we prepared a composite that was characterized by different physico-chemical analysis methods.

The second part of this study focused on the removal and degradation of methylene blue (MB) in aqueous solution by this composite, and the influence of certain experimental parameters on the adsorption capacity of (MB) was studied, including the effect of contact time, the pH of the solutions, the initial concentration and temperature, as well as the photocatalytic degradation under solar irradiation. The adsorption results show that the kinetics of the pseudo-second-order model and the Langmuir isotherm correspond well to the experimental data [2].

Key words: Nonlinear optical materials (NLO), Copolymer, Activated clay Mg-H+, Composite, Adsorption, Methylene Blue (MB) Dye.

Corresponding Email: imene.arbouz@univ-sba.dz

References

P-054

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Analysis of adsorption of Congo red dye onto trioctylmethylammonium modified Algerian bentonite using Box-Behnken design approch

Brahim GUEZZEN [a*], Rachida BERREZOUK [b] and Baghdad MEDJAHED [a]

[a] Laboratory of Separation and Purification Technology, Department of Chemistry, Faculty of Sciences, Tlemcen University, Box 119, Algeria. Department of Process Engineering, Faculty of Technology, Dr. Moulay Tahar University, Saida, Algeria

[b] Laboratory of Physico-chemical Studies, Department of Chemistry, Faculty of Sciences, Dr. Moulay Tahar University, Saida, Algeria

Abstract:

The aim of this research was to evaluate the efficiency of trioctylmethylammonium modified Algerian bentonite as an adsorbent for Congo red (CR) adsorption from aqueous solution by using Response Surface Methodology (RSM). The process parameters, namely temperature, adsorbent dosage, and initial dye concentration on the removal of CR were optimized using Box-Behnken design (BBD). The results demonstrate that all these factors are statistically significant, including the interactive effect of adsorbent dosage and initial dye concentration. The F-value and P-value of the fitted second order model were obtained as 202.21and 0.0001, respectively. The experimental and predicted values were within 95% confidence interval, which demonstrates that the second-order polynomial model can successfully predict the efficiency of CR removal using modified bentonite. At the optimized condition, the maximum CR adsorption was found to be 89.3 %. The test results indicated trioctylmethylammonium modified bentonite could be important from the perspective of performance and affordability.

Key words: Trioctylmethylammonium modified bentonite, Congo red, Adsorption, Box–Behnken design

P-055

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Ab-initio study of $TlGeX_3$ (X= Br, Cl) for photovoltaic applications

MEKHALEF BENHAFSA Leila[a], AZZAZ Yahia[b], BELLAHCENE Fatima Zohra Zoulikha[c], BERROUNA Henen[d]

[a,c] Faculty of Sciences and Technology, University of Belhadj Bouchaib - Ain Temouchent, Laboratory of the Magnetic Materials - Sidi Bel Abbes, Algeria
[b,d] Faculty of Exact Sciences, University of Djillali Liabes - Sidi Bel Abbes, Laboratory of Physics and Chemistry of Advanced Materials, Algeria

Abstract:

Recent research has shown great interest in halide perovskites due to their excellent optoelectronic properties. In the present work, the structural, elastic, electronic and optical properties of cubic halide perovskite $TlGeX_3$ (X= Br, Cl) compounds are investigated by using the full potential linearized augmented plane wave (FP-LAPW) method[1] based on density functional theory (DFT). The exchange and correlation potentials were treated by the generalized gradient approximation (GGA-PBE)[2] in the process of energy optimization. Moreover, the modified Beck Johnson potential approach parameterized by Tran-Blaha (TB-mBJ)[3] was used to calculate the electronic and optical properties. The calculated elastic parameters suggest that these compounds are mechanically stable and ductile. Subsequently, the results achieved for the electronic properties show that both compounds are semiconductors with a direct band gap along [R-R], which are appropriate for solar cell applications. These compounds also possess attractive optical properties, notably a good absorption coefficient in the visible and ultraviolet region, making them promising candidates for photovoltaic and other optoelectronic applications.

Key words: Halide perovskites, DFT, Optoelectronic properties, Elastic properties

P-056

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Title: Stability Analysis of SnO_2 Thin Film Gas Sensors Using tools (AES, EELS and AFM)

Zakia Lounis[a], M-Salah halati [a,b], Moussaab Belarbi[c], Malika Achouri[a]

[a] Laboratory of Materials (LabMat), National Polytechnic School of Oran, ENPO-MA,Oran Algeria
[b]Scientific and Technical Research Centre for Arid Areas C.R.S.T.R.A Omar El Barnaoui, Campus of Mohamed, Khider University of Biskra, 07000, Algeria
[c] Laboratory of Micro and Nanophysics (LaMiN), National Polytechnic School Oran, ENPO-MA

Abstract:

This study investigates the surface stability of SnO2 thin films, commonly used as gas sensors in industrial applications. Samples, synthesized using the spray pyrolysis method at different substrate temperatures (300°C, 340°C, and 380°C), were analyzed at different temperatures underwent repeated heating cycles and Argon ion bombardment. Carbon diffusion and oxygen increase were observed, detected by Auger Electron Spectroscopy (AES) and Electron Energy Loss Spectroscopy (EELS). Argon beam bombardment caused desorption of carbon and oxygen. A third heating cycle aimed to restore surfaces and modify stoichiometry, confirmed by AES and EELS signatures. Atomic Force Microscopy (AFM) analysis validated surface morphology changes. Overall, the study highlights the surface stability of SnO2 thin films.

Key words: Gas sensor, SnO_2 thin-film, AES, EELS spectroscopy , AFM microscopy, surface stability, absorption and desorption.

Corresponding Email: zakia.lounis@yahoo.fr, zakia.lounis@enp-oran.dz

---

References

[1] Zakia Lounis, M'hamed Bouslama, et al. *Journal of Electron Spectroscopy and Related Phenomena* 226, 9-16, 2018

[2] Djamel Ghaffor, Zakia Lounis, et al, *Journal of Materials Science Materials in Electronics 31(2–4), May 2020*

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Structural, Electronic, and Elastic Properties of New Halid Peroveskite (RbRaI3) from Ab initio Calculation.

A. Douma Bouthiba[1], A. Adjadj[1, 2]

[1]Laboratoire de Génie physique, University of Tiaret, 14000 Alegria.
[2]Faculty of Science and technology, University Belhadj Bouchaib, Ain-Temouchent,46000 Algeria.

Abstract

This study aims to provide a thorough analysis of Rubidium Radium Iode (RbRaI3), a lead free and non-toxic type of perovskite. The investigation is primarily focused on its structural, electrical and mechanical properties. Density functional theory (DFT) is combined with the Full-Potential Augmented Plane Wave (FP LAPW) method found in the WIEN2k code for this analysis. The electronic properties are studied in detail using two different approximations: the structural features are adjusted using the generalized gradient approximation (GGA) and the semiconductor behavior is verified using the modified Becke-Johnson potential (mBJ). The compound's stability is demonstrated by the computations' negative formation energy values. Moreover, the mechanical stability is confirmed through the elastic parameters such as shear modulus (G), Bulk modulus (B), Poisson ratio (ν) and Cauchy pressure among other elastic coefficients .

Keywords: FP -LAPW,Wien2k , peroveskite, RbRaI3 ,structural, electronic, elastic.

P-058

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Title: Catalytic behavior and antibacterial/antifungal activities of new MNPs/zeolite@ alginate composite beads

Amel Mekki [a], Fadhila Bouhella [b], Mohammed Hachemaoui [c], Adel Mokhtar [d], Farid Bennabi[e], Khaled Rahmani [e], Bouhadjar Boukoussa[f].

[a] Materials chemistry laboratory, University of Oran1 Ahmed Ben Bella ,Oran ,Algeria
[b] Sciences and Technologies Process Engineering laboratory, university of sciences and technologies of Oran, Algeria
[c] Department of materials sciences , University of Oran1 Ahmed Ben Bella ,Oran,Algeria
[d] Department of process Engineering ,Institute of science and technologies, University of Ahmed Zabana, Relizene ,Algeria
[e] Department of biology ,University of Ain-Temouchent Belhadj Bouchaib , Ain-Temouchent ,Algeria
[f] Department of Materials Engineering, university of sciences and technologies of Oran, Algeria

Abstract:

In this paper, a new family of composite materials was prepared based on calcium alginate and metal nanoparticle-loaded zeolite omega. Different types of metal nanoparticles (MNPs), namely Cu, Co and Fe, were loaded onto zeolite omega to test the performance of the resulting metal/zeolite@alginate composites towards the catalytic reduction of methylene blue dye. To examine their application field as broadly as possible, these composite beads were also tested as antibacterial and antifungal agents against several types of bacteria. Several techniques such as XRD, XRF, FTIR, XPS, SEM and TGA were used to characterize the samples. The obtained results showed that all the composite bead samples were effective in the reduction of MB dye. The composite Co/Zeolite@ALG with relatively low Co nanoparticle (NP) content was selected as the best performing catalyst due to its reduction of MB dye being completely achieved in 3 min with a rate constant of 1.4 min−1, which was attributed to its highly porous structure. The reuse tests conducted on the best-performing catalyst showed good results which persisted through five successive cycles. For antibacterial

and antifungal activities, the Cu/Zeolite@ALG and Fe/Zeolite@ALG composites showed good activity with significant inhibition zones.

Key words: Zeolite ,catalytic reduction , methylene blue dye , antibacterial and antifungal activities.

Corresponding Email: bouhellabouhella2022@gmail.com & bbouhdjer@yahoo.fr

References

[1] B. Boukoussa et al.Adsorption behavior of cationic dye on mesoporous silica SBA-15 carried by calcium alginate beads: Experimental and molecular dynamics study,J. Mol. Liq.(2021)

[2] M. Hachemaoui et al.Composites beads based on Fe3O4@MCM-41 and calcium alginate for enhanced catalytic reduction of organic dyes,Int. J. Biol. Macromol.(2020)

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Inter-Satellite Simulation with Custom Modulation: Enabling DVB-RCS2 Integration with Optical Communication Networks

Meryem Romaissa DJELLOULI[a], Sid Ahmed CHOUAKRI[b], Abdelkrim GHAZ[c]

[a]Meryem Romaissa DJELLOULI, Telecommunications, Djillali Liabes, Sidi Bel Abbes, Algeria
[b]Sid Ahmed CHOUAKRI, Telecommunications, Djillali Liabes, Sidi Bel Abbes, Algeria
[c]Abdelkrim GHAZ, Telecommunications, Djillali Liabes, Sidi Bel Abbes, Algeria

Abstract:

The updated technical report outlines a GEO-type inter-satellite connectivity, operating at a data rate of 300 Gbps, with a subsystem input power of 30 dBm. This connectivity is based on laser optical communication (OWC), with a focus on more specific modulations such as QPSK and 16-QAM, implemented using Optisystem software. Performance measurements include Q factors of 2271, 1734, 15.9248 and 14.356 dB, as well as bit error rates (BER) of 0, 2.00575×10^{-057}, and 4.86113×10^{-047}. This approach highlights the importance of robust technical support for the recent DVB-RCS2 satellite standards, aimed at improving two-way telecommunications services.

Key words: Is-OWC, GEO, 16-QAM, QPSK, DVB-RCS2, OptiSystem.

Corresponding Email: meryemromaissa1@gmail.com

References

[1] M. Faugerona A. Mahoa, "Assessment of the effective performance of DPSK vs. OOK in satellite based optical communications," In International Conference on Space Optics, Chania, Greece, 9 - 12 Octobrer 2018.
[2] Arun Prakash, S., Sumithra, M.G., Shankar, K. et al. Performance investigation of spectral-efficient high-speed inter-satellite optical wireless communication link incorporating polarization division multiplexing. Opt Quant Electron 53, 270, 2021.

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Investigating the Structural and Electronic Properties of AlN/GaN Superlattices Along (110), (110), and (111) Growth Axes Using First Principles

Deloum Amira; Mimouna Oukli; Abid Hamza

[a]Applied Materials Laboratory (A.M.L), Faculty of Electrical Engineering, Djillali Liabes University of Sidi Bel Abbes, 2200 Sidi Bel Abbes, Algeria.

Abstract:

In this study, we employ first-principles calculations to investigate the structural and electronic properties of AlN/GaN zinc-blende/zinc-blende superlattices. Our approach involves utilizing the full potential linear muffin-tin orbitals (FPLMTO) method within the plane wave approximation (PLW). This method offers accurate treatment of interstitial regions and avoids the reliance on adjustable parameters, ensuring a reliable and microscopic analysis. We explore the AlN/GaN superlattices in three different growth directions: (001), (110), and (111). By calculating the electronic structures of these superlattices, we compare and analyze their properties. Our investigation includes examiningthe partial density of states, which allows us to understand the changes in the nature of the band gaps observed in the (110) and (111) growth axis superlattices. We find that these modifications can be attributed to the strong hybridization of the Ga and N atoms' pd and sp orbitals.

Key words: AlN ; GaN ; 110 and 111 growth axis ; Superlattices ; Electronic structure

Corresponding Email: amiradelloum28@gmail.com

P-061

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Theoretical investigation of structural, mechanical, and thermodynamic properties of HfX_2 (X=S, Se) using first-principles calculations

Khatir OUAIL[a], Samia FERAHTIA[a], Salima SAIB[a]

[a] Laboratory of Materials Physics and its Applications, Physics Department, Faculty of Sciences, University of M'sila, Algeria

Abstract:

Nowadays, due to the growing use of energy in modern life, it has become an urgent necessity to search for environmentally friendly energy resources and reduce dependence on fossil fuels and conventional energy sources and the consequent carbon emissions. Solar energy is a notably effective renewable power source; however, its performance is based on the improvement of photovoltaic materials [1, 2]. Recently, transition metal dichalcogenides (TMDCs) have received considerable attention from researchers and scientists as a type of two-dimensional (2D) material because of their electronic, optical, mechanical, and thermal properties and their potential applications in electronic and solar energy-harvesting devices [2, 3]. TMDCs are van der Waals multilayer semiconductors of kind MX2, with M representing a transition metal atom like Hf, Mo, or W and X representing a group-16 element like S or Se [2, 4]. In this work, we focus on two simple TMDC materials, HfX_2 (X = S and Se). These materials exhibit high optical absorption in the visible spectrum and semiconducting behavior in both experimental and theoretical band gaps. Accordingly, HfX_2 (X = S, Se) can be further used as potential components in optical absorbers for next-generation solar cells [1].

Kohn–Sham density functional theory (DFT) with vander Waals forces proposed by Grimme [5] has been used to study the structural, mechanical, and thermodynamics properties of HfX_2 (X=S or Se) in P–3m1 structures. All the first-principles calculations are performed using the ABINIT code and taking into account the van der Waals interaction by the empirical dispersion correction using the method of Grimme (DFT (PBE)-D3). Perdew-Burke-Ernzerhof (PBE) functional form of generalized gradient approximation (GGA) has been used for the exchange and correlation of electrons, and projector augmented wave(PAW). All the transition metal

dichalcogenides (TMDCs) under investigation exhibit significant elastic anisotropy and layered structural features. Our results indicate that the HfS2 and HfSe2 compounds are reasonably machinable and moderately hard. Furthermore, the GIBBS 2 code was utilized to explore the temperature dependence of specific macroscopic parameters within the framework of the quasi-harmonic model of Debye.

Key words: Transition metal dichalcogenides, van der Waals corrections, Mechanical properties, thermodynamics properties.

Corresponding Email: khatir.ouail@univ-msila.dz

References

[1] D. Singh, R. Ahuja, ACS Applied Energy Materials 2, 6891(2019)

[2] Ruotong Zhang et al, J. Phys. D Appl. Phys 55, 295304(2022)

[3] A. Mashmool, et al, J. Magnetism and Magnetic Materials 503, 166572(2020)

[4] J. Ibáñez, T.Woźniak, F. Dybala, R. Oliva, S. Hernández, R. Kudrawiec, SCIENTIFIC REPORTS 8, 12757(2018)

[5] S. Grimme, J. Comput. Chem. 25, 1463(2004).

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Multilayer Perceptron using Molecular Descriptors to model the Essential Oil Yield from Medicinal Herbs

Ilhem Bouaziz [a], Mohamed Hentabli [a], Mohamed Kouider Amar [a], Ahmed Chabane[b], and Salah Hanini[a]

[a] Biomaterials and Transport Phenomena Laboratory, Faculty of Technology, University Yahia Fares of Medea 26000, Medea, Algeria.

[b] Laboratoire des Matériaux Organiques (LMO), Département de Génie des Procédés, Faculté de Technologie, Université de Bejaia, 06000 Bejaia Algérie.

Abstract:

This research investigates the predictive potential of Multilayer Perceptron (MLP) Neural Networks utilizing Molecular descriptors to estimate the yield of essential oils from samples of Medicinal Herbs. We propose an innovative method by generating molecular descriptors for the primary components of Herbs and processing them through an autoencoder. The encoded data, along with experimental parameters, are then merged with an MLP to enhance accuracy. Drawing from data acquired through previous investigations, we utilized a dataset comprising 300 samples from 15 distinct medicinal plants, employing the Supercritical Fluid Extraction method. The outcomes reveal a remarkably high R^2 value approaching unity, indicating a robust correlation between actual and predicted yields. Additionally, the Root Mean Squared Error was calculated to be 0.96%.

Key words: Molecular descriptors, Multilayer Perceptron, Essential Oil Yield, Medicinal Herbs.

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Exploring Green Solvents for the Separation of Imidacloprid from Aqueous Environments: A Theoretical Study on Behavior, Stability, and Environmental Implications

M. Hammar[a,b], N. Benbrahim, A. Negadi[b]

[a] Laboratory of Advanced Materials and Physicochemistry for Environment and Health, Djillali Liabes University, Sidi Bel Abbes, Algeria.
[b] Laboratory of Thermodynamics and Molecular Modeling, Abou Bekr Belkaid University, Tlemcen, Algeria.

Abstract:

This theoretical study investigates the interaction of the insecticide imidacloprid, or 1-[(6-chloro-3-pyridinyl)methyl]-4,5-Dihydro-N-nitro,1H-Imidazol-2-amine, with two green solvents to propose effective solutions for its separation from aqueous media [1].

Using B3LYP/6-31G(d,p) density functional quantum mechanical method and Gaussian09 software, the structures of imidacloprid were calculated and compared in gaseous, aqueous, and organic solvent environments. The study explores the stability of imidacloprid in various solvents and their mixtures, providing insights into its behavior, stability, and toxicity. The values will be compared to curves previously obtained by N. Benbrahim & al. [2].

The results highlight the preference of imidacloprid for aqueous media and reveal an inverse stability trend in solvent mixtures with different fractions. The calculated descriptors include electronegativity, chemical potential, chemical hardness, chemical softness, and electrophilic index. The findings contribute to a deeper understanding of imidacloprid's behavior in different environments, offering potential strategies for its purification from surface water traces using green solvents [3].

Keywords: Imidacloprid, Density Functional Theory, Green solvents, Water Purification.

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Exploring the Structural, Electronic Properties and Reactivity of Benzimidazole derivative in Solvent Environment using DFT Study

Noreya BESTAOUI-BERREKHCHI-BERRAHMA, Chaimaa KHERBABA

Faculté des Sciences Exactes, Laboratoire de Chimie Théorique de Bio & Nanosystème LCTBN, Université Djillali Liabes de Sidi Bel Abbès, B.P.89, Sidi Bel Abbès, 22000, ALGERIE

Abstract:

In recent decades, heterocyclic chemistry has experienced significant growth, leading to the synthesis of numerous compounds featuring at least one heterocyclic ring in their structure. Heterocycles serve as fundamental frameworks for a diverse range of chemical, biological, pharmacological, industrial, and therapeutic compounds, including vitamins, hormones, antibiotics, and more. They also play crucial roles in industrial and technological applications, such as corrosion inhibitors, dyes, stabilizing agents, pesticides, and herbicides. Nitrogen, a common element within heterocycles, is found in many naturally occurring pharmacologically active molecules. As a result, various methods have been developed to synthesize nitrogen-containing compounds, with a particular focus on heterocyclic molecules.

In this study, we explore the properties of the 6-aminobenzimidazole molecule within a solvent environment. Using quantum chemical calculations employing density functional theory (DFT), we employed the B3LYP functional and Aug-cc-pVDZ basis set. The implicit solvent was chosen, with the Polarizable Continuum Model (PCM) implemented for simulation. Computational analyses were conducted using the Gaussian 09 program.

The NBO (Natural Bond Orbital) analysis enabled a comprehensive examination of all orbital interactions within the compound. Additionally, we computed both global (χ, μ, η, ω, S, and εHOMO, εLUMO) and local (Fukui indices (f+, f-), local softness (S+, S-), and local electrophilic powers (ω+, ω-)) reactivity descriptors. These calculations were crucial in identifying the reactive sites within the molecule and assessing its susceptibility towards electrophilic and nucleophilic attacks.

Key words: DFT Method, chemical reactivity, HOMO-LUMO, global and local reactivity descriptors, electrophilic and nucleophilic attacks.

P-065

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Influence Analysis of the Ambient Conditions on the Vortex Tower Prototype Performance

A. Bouam*[a], A. L. Cheridi Deghal[b], A. Dadda[b], A. Hadjam[a], N. Koudiah[c], K. Attari[a], A. Dahia[a]

[a]Nuclear Technology Division, Nuclear Research Centre of Birine, P.O. box 180 Ain-Oussera, Algeria.
[b]Nuclear Safety and Radiation Protection Division, Nuclear Research Centre of Birine, P.O. box 180 Ain-Oussera, Algeria.
[c]Electronics and Nuclear Instrumentation Development Division, Nuclear Research Centre of Birine, P.O. box 180 Ain-Oussera, Algeria

Abstract:

Because of the depletion and the harmful effects of the conventional resources of energy, the need for the developments of the renewable energy system has become essential. The cooling of a nuclear power plant can only be done through the cooling towers and following the insufficient of water supplying this equipment, we propose in this study to couple a classic cooling tower with a Vortex Tower (VT). This equipment improves the performance of the nuclear power plants, saves water resources, reduces thermal pollution and contributes to electricity production in a country. The simulation results clearly show the capacity of the Vortex Tower Prototype (VTP) to produce an upward air current surrounded by an artificial vortex [1].

The performances of all VTs are affected by changes in Ambient Conditions (AC). Variations in temperature, pressure and humidity generally exert the biggest influence while winds, inversions, rain, snow, hail and solar radiation have a less significant effect. So, the main purpose of this study is to analyze the influence of ambient conditions on the performance of the VTP.

Our work starts by the mechanical conception of the VTP on a laboratory scale [2]. The heat source used is a coaxial cylindrical tank (ring type) filled with water and heated by electrical resistances. The air circulation inside the VTP is due to the difference of the density and the role of the artificial vortex is to accelerate the cooling of the air.

In this work, several experiments were carried out. The measurements were recorded in periods where the ambient conditions were different. Three days are considered (6 march, 10 march and 13 march).
Several results were recorded from these experiments; it was found that the velocity of the upward airflow is inversely proportional to the outlet temperature (ambient temperature). It was also found that the air velocity measured at the chimney inlet is inversely proportional to the humidity of the climate. The efficiency of this equipment is inversely proportional to the ambient temperature, which is verified by Carnot cycle. It was found that the low variations ambient pressure effects of on VTP are negligible. In conclusion, both ambient temperature and humidity affect the VTP performance.

Key words: Vortex tower prototype (VTP), Artificial vortex, Ascendant air flow, Ambient conditions.

Corresponding Email: a.bouam@crnb.dz, bouam05_ab@yahoo.fr

References

[1]- A. HADJAM, A. DAHIA, A. L. DEGHAL CHERIDI, A. BOUAM, A. DADDA, K. ATTARI, N. KOUDIAH, A. GHADBANE, *"Numerical analysis of a small-scale novel vortex tower integrated with heat source for Nuclear Application"*, Nuclear Engineering and Design 414 (2023) 112660, https://doi.org/10.1016/j.nucengdes.2023.112660.

[2]- A.L. DEGHAL CHERIDI, A. DADDA, A. BOUAM, N. KOUDIAH, A. DAHIA & K. ATTARI, *"Realization and experimentation of a novel vortex cooling tower"*, Energy Conversion and Management, 270 (2022) 116197, https://doi.org/10.1016/j.enconman.2022.116197.

.....

P-066

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Title: Ab-initio investigation of structural, electronic, magnetic and optical proprieties of a novel double perovskite: Sr2CeRuO6

Fatima Zohra Zoulikha Bellahcene [a,b,c], Leila Mekhalef Benhafsa[a,b], Kaddour Bencherif[a,c], Fafa Chiker [c].

[a] Faculty of Sciences and Technology, University of Ain Temouchent, Belhadj Bouchaib,Algeria .
[b] Laboratory of the Magnetic Materials, Faculty of Sciences Exacts, University of Djilali Liabes, 22000, Sidi Bel Abbes, Algeria.
[c] Laboratory of Study of Materials and Optical Instruments, Faculty of Sciences Exacts, University of Djilali Liabes, 22000, Sidi Bel Abbes, Algeria

Abstract:

In this study, we investigated the structural, electronic, magnetic, and optical properties of the double perovskite Sr2CeRuO6. Utilizing the linearly augmented plane wave method with total potential (FP-LAPW)[1], within density functional theory (DFT), implemented in the Wien2k code [2]using the generalized gradient approximation (GGA), we confirmed the stability of this new material by optimizing its structure and tolerance factor. Additionally, we found that the compound is more stable in the ferromagnetic order than in the non-magnetic order. Our study of the electronic band structures and density of states revealed that the compound under investigation exhibits half-metallic behavior with significant energy band gaps, indicating its electronic stability. Analysis using the modified Becke –Johnson potential showed that the studied compound has an indirect band gap from X to Γ with values of 1.7986 eV for the majority spin and metallic behavior for the minority spin.
Additionally, we conducted an assessment of the compound's optical properties, including analysis of the real and imaginary parts of the dielectric function and the refractive index. These findings offer insights into potential applications across diverse scientific and technological domains.

Key words: Density functional theory, Optical properties, magnetic proprieties, double perovskite

P-067

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Synthesis of a hybrid material-Organophosphazene- catalyzed by clay(Maghnite-H^+)

'MEDJDOUB Lahouaria[a], BENNABI Souad[b]

[a]MEDJDOUB Lahouaria' Higher School of Biological Sciences of Oran (ESSBO) – Algeria.
[b] BENNABI Souad' Hassiba Ben Bouali University, Chlef, Algeria.

Abstract:

Phosphazenes are inorganic compounds that belong to the most important class of cyclic or linear structures based on phosphorus with the general formula $(R_2P=N)n$. Most phosphazene structures are easily synthesized by aminolysis of phosphorus pentachloride, PCl_5. Nucleophilic substitution on hexachlorocyclotriphosphazene leads to hybrid compounds (organic-inorganic): organophosphazenes. Nucleophilic substitution on hexachlorocyclotriphosphazene by piperazine was performed for the first time under mild conditions and in the presence of an eco-catalyst: Maghnite-H^+[1,2]. The role of the catalyst holds industrial importance, favoring the use of Maghnite which has many advantages: a very low purchase price compared to other catalysts, easy removal of the reaction mixture. Maghnite becomes an excellent catalyst for several chemical reactions. The obtained product was characterized by 1H MAS NMR, 15N MAS NMR, IR, and TG.

Key words: Hexachlorocyclotriphosphazene, Piperazine, Organophosphazene, Maghnite-H^+, RMN.

Corresponding Email:

houariamejdoub@yahoo.fr

References

[1] M.Belbachir, U.S.Patent. 066969.0101-**2001**.
[2] M.Belbachir, A.Bensaoula ; US Patent. **2006 ;** 7, 094, 823.

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

The internal repair by bonding the composite patch

GHRIBI Saadiaa[a], M'hamdia Rachid[a]

[a] LMPA, departement of Mechanical Engineering, University of Technology, Sidi Bel Abbes , Algeria

Abstract:

Recently, bonded composite patch repair of structures has become an increasingly popular and promising technology. Among the repair techniques, we find the internal repair by bonding techniques using composite materials. In this study, an internal repair of a cracked plate was carried out to increase its service life, with a study analyzing its cracking behavior before and after internal repair using a laminate boron/epoxy composite material. The aim of this experimental study is, of course, to arrive at a point where the lowest possible stress lies on the repair plate. The results enable us to consider the internal composite bonded repair we carry out as the best performer in composite repair.

Key words: plate cracked, internal repair by bonding, composite patch.

Corresponding Email: *saadia.ghribi@univ-sba.dz*

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Physicochemical properties of nanocrystalline cellulose isolated from artichoke microcrystalline cellulose

Moufida BEROUAL[1]*, Fawzia BOURSAS [2], Maroua BENLEMBAREK [3].

[1]Laboratory of Macromolecular and Macromolecular Thio-Organic Synthesis, Faculty of Chemistry, USTHB, BP32, 16111 Algiers, Algeria
[2]Department of Chemistry and Physics of Inorganic Materials, Faculty of Chemistry, USTHB, BP32, 16111 Algiers, Algeria
[3]Laboratory of Natural Gas Chemistry, Faculty of Chemistry, USTHB, BP32, 16111 Algiers, Algeria
*E-mail Address: moufidaberoual@gmail.com

Abstract

Inasmuch, this paper is desired to encourage the emergence of preparation of cellulose nanocrystals with controlled morphology, structure and properties, so that enable positive development of biocompatible, renewable and sustainable reinforcing materials for polymer composites field. Increased solicitude towards "green chemistry" drew scientists and scholars' heed to utilize eco-friendly polymers to denigrate the ecological risks generated by typically used petroleum raw material. The exceptional mechanical and chemical characteristics of cellulose nanocrystal composites enable the effective utilization of cellulose nanocrystal composites in diverse prospective than remaining cellulosic derivatives. The present work dedicated on the isolation of commercial nanocrystalline cellulose (CNCC) from artichoke microcrystalline cellulose (AMCC) using acid hydrolysis method. The obtained sample was characterized using infrared spectroscopy (FTIR), X-ray diffraction (XRD), scanning electron microscopy (SEM).The FTIR spectroscopy exhibited the increase of crystalline peak, which is referred to CH2 symmetric stretching in ANCC sample indicating the removal of the amorphous regions. The XRD data showed that the NCC sample have higher crystallinity index about 92.45 % higher than of MCC 72.33 % with cellulose I structure. From SEM

images, it is clear that the different NCC particles presented rough surface and nano-sized particles between 77 and 129 nm. Consequently, based on these findings, the commercial nanocrystalline cellulose fibers can be isolated from AMCC and used as a promising resource in outstanding features.

Keywords: Cellulose, artchoke nanocrystalline cellulose, microcrystalline cellulose, acid hydrolysis, eco-friendly polymers.

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Source term calculation and risk evaluation during accidental release of BWR Nuclear Reactor

A. Dahia, A. Dadda, A. L. C. Deghal, A. Bouam

Nuclear Research Centre of Birine, B.P 180 Ain Oussera 17200, Djelfa, Algeria

Abstract:

In this paper, we estimate the radionuclide inventory of BWR Nuclear Power Plant core operating at 36 months in several power of 1356 MWe, considering a release of 137Cs to the environment. The calculations were performed based on the ORIGEN JR code. The Total Effective Dose (TED), the time-integrated air concentration, and the ground deposition are consequently determined for more instable atmospheric stability class "A" using health physics HotSpot code. Follow this, a comparative study has been done considering two scenarios for simulation, General Fire and General Explosion. Hence, the total dose distributions on human organs were also computed and compared to the authorized dose limits.

Key words: Radionuclides, TED, Radiation dose, Gaussian model.

Corresponding email: a.dahia@crnb.dz / dahia.univ@gmail.com

P-071

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Étude numérique du facteur d'intensité de contrainte dans les structures navales endommagées par fissuration

M.S.N. BOUSSAHRA[a], S. LIAMANI[b], M. BAGHDADI[b], I. LARICHE[c], B. SERIER[c]

[,a] Laboratoire de Mécanique Physique des Matériaux : Faculté de Technologie, Université Djillali Liabes de Sidi Bel-Abbes
[B] Auteur correspondant : Sidi Bel Abbes, Algérie.

[c] Pr émérite Laboratoire de Mécanique Physique des Matériaux : Faculté de Technologie, Université Djillali Liabes de Sidi Bel-Abbes

Résumé:

Les patchs composites sont largement utilisés pour réparer les structures endommagées par fatigue ou autres. Ces patchs permettent de retarder la propagation des fissures et par conséquent d'augmenter la durée de vie des structures ainsi réparées. Beaucoup de travaux ont été consacrés à l'étude numérique du comportement mécanique de la réparation par patchs composites collés [1-10]. Ainsi, l'effet de plusieurs paramètres physiques et géométriques sur la performance et l'efficacité de la réparation en termes de réduction du facteur d'intensité de contrainte. Cette étude rentre dans cet objectif et vise à analyser la performance de la réparation en termes de réduction du FIC.

La réparation par patch composite initialement appliquée pour le renforcement des structures aéronefs vieillissant et fissurée est actuellement généralisée à d'autres secteurs industriels et notamment dans le domaine des structures navales. Cette étude rentre dans ce contexte et a pour objectif la contribution à l'amélioration de la performance des composants navals endommagés par fissuration en termes de réduction du FIC en mode I et mode II.

MOTS CLES : FIC, Fissure, Mode I, MODE II, Patch, Adhésif

P-072

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Adsorption of cationic dyes using surfactant modified algerian clay : kinetic and adsorption mechanism studies.

Marwa Jdidi[a,b], Amina Sardi [a,c] ,Boumediene Bounaceur[a], Néji Besbes[b].

[a]Macromolecular Physical Chemistry Laboratory, Department of Chemistry, University Oran1, AB. P.O. Box 1524, Oran, 31000, Algeria.

[b]Laboratory of Composite Materials and Clay Minerals, Group of Green and Applied Organic Chemistry, National Center for Research in Materials Science, Technopole of Borj Cedria, Soliman, B.P 73, 8027, Tunisia.

[c]University Hassiba Ben Bouali, Faculté Science Exacte et Informatique, Département de Chimie, Ouled Fares, 02010 Chlef, Algeria.

E-mail: Jmarwa359@gmail.com, b_bounaceur@yahoo.fr, besbesneji@yahoo.fr, a.sardi@univ-chlef.dz

Abstract

The present study describes the preparation of new eco-friendly adsorbents with a simple method. frst, Montmorillonite (MMT) [1] was modifed with hexadecyltrimethylammonium bromide surfactant HTAB (MMT@HTAB) [2] and then with polymer PolyVinylAlcohol (PVA) (MMT@HTAB@PVA) [3]. The as-synthe sized materials were characterized by several characterization techniques, including X-ray diffractin (XRD), Fourier-transform infrared spectroscopy (FTIR), Scanning electron microscopy (SEM), Thermogravimetric analysis (TGA) and zeta potential measurement then evaluated as adsorbents for removal of methylene blue (MB) as a cationic dye from aqueous solution under different contact time, dye concentration and pH [4]. The obtained results confirm the intercalation of surfactant within the clay layers, while the obtained nanocomposite showed different morphologies and structures in which the exfoliated and intercalated forms were obtained [5]. The adsorption kinetics of MB on MMT@HTAB@PVA was best fetted by the pseudo-second order model, The thermodynamic study showed that the adsorption processes of MB by the both MMT@HTAB and MMT@HTAB@PVA adsorbents occur in an

autonomous way and the tem perature has not a signifcant effect on the adsorption capacity of MB dye [6].

Keywords : Modified clay, Intercalaion, cationic dye, surfactant, Polymer

References :

[1] : Taher T, Munandar A, Mawaddah N et al (2023) Synthesis and characterization of montmorillonite – Mixed metal oxide composite and its adsorption performance for anionic and cationic dyes removal. Inorg Chem Commun 147 :110231. https://doi.org/10.1016/j.inoche.2022.110231

[2] : Sardi A.; Bounaceur B.; Mokhtar A.; Boukoussa B.; Abbes M. T; Chaibi8 W.; Nacer A.; Brahma Khadidja K.; Issam I.;· Jibran Iqbal J.; Patole S. P.; Abboud M. Kinetics and Thermodynamic Studies for Removal of Trypan Blue and Methylene Blue from Water Using Nano Clay Filled Composite of HTAB and PEG and its Antibacterial Activity, J. Polym. Environ., https://doi.org/10.1007/s10924-023-02927-6 ;3 Juin 2023

[3] : Brown K, Mendoza M, Tinsley T et al (2021) Polyvinyl alcohol-montmorillonite composites for water purification : Analysis of clay mineral cation exchange and composite particle synthesis. Polyhedron 205 :115297 . https://doi.org/10.1016/j.poly.2021.115397

[4] : Kathiresan G,VijayaKumar K, Sundarrajan AP et al (2021) Photocatalytic degradation efficiency of ZnO, GO, and PVA nanoadsorbents for crystal violet, methylene blue and trypan blue dyes. Optik 238:166671. https://doi.org/10.1016/j.ijleo.2021.166671

[5] : Belbel A, Kharroubi M, Janot J-M et al (2018) preparation and charactterization of homoionic montmorillonite modified with ionic liquid : application in dye adsorption. Colloids Surf, A558 :219-227.https://doi.org/10.1016/j.colsurfa.2018.08.080

[6] : Zhang L-L, Zaoui A, SeKKal W, Zheng Y-Y (2023) Interlayer adsorption of cationic dye on cationic surfactant-modified and unmodified montmorillonite. J. Hazardous Mater. 442 :130107.https://doi.org/10.1016/j.jhazmat.2022.130107

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Numerical Simulation of The Mechanical Behavior and Feasibility of a Hip Prosthesis Architecture.

Badi ridha, Mokhtari Ahcen, Masmoudi youcef Amine, Brick chaouche Amine, Tala Ighil N.

Research Center in Industrial Technologies (CRTI), P.O. Box 64, Chéraga 16014

Abstract:

The implantation of hip prostheses is a lifesaving intervention for many patients suffering from severe joint problems. Thanks to technological and surgical advancements, this procedure offers highly satisfactory results, enabling patients to regain a better quality of life and resume their daily activities with increased comfort and mobility. Current prostheses consist of a femoral component (a ball attached to a stem) and a part implanted in the iliac bone (a cup, in which the ball fits). The ball rotates within the cup with friction, sometimes significant due to the stresses corresponding to the body's weight. Orthopedic surgeons carefully assess each patient's case to determine the most suitable prosthesis type tailored to their specific needs. The goal is to explore various alternative designs that align with functional specifications, aiming to streamline the placement of hip prostheses and improve their mechanical performance.

Key words: Wear debris, Articulation, Hip prosthesis, *Simulation.*

Corresponding Email:r.badi@crti.dz

P-074

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Reinforcement of the properties of biodegradable PLA-based films by integration of nanoparticles and bioactive agent

Rebiha BENCHERIk and Assia Siham HADJ-HAMOU

University of Sciences and Technology Houari Boumediene, Laboratory of Polymeric Materials, Macrolecular Chemistry Department, Faculty of Chemistry, BP 32, 16111 El Alia, Bab Ezzouar, Algiers, Algeria.

Abstract:

The food packaging sector is known to be one of the most active areas of research development and a great technological interest in the field of nanoscience, which requires significant investments from industrialists and governments.

The food packaging sector is recognized as one of the most dynamic fields for research and development, attracting considerable technological interest within nanoscience. This focus requires significant investments from both industry leaders and government bodies.

In our research, we used PLA to develop bionanocomposite films with improved properties suitable for food packaging. Our goal was to reinforce the PLA matrix by incorporating a small amount of ZnO nanoparticles along with a bioactive agent (ATH). These nanocomposites were then developed and rigorously characterized using various techniques.

The addition of ZnO NPs-ATH to the PLA matrix significantly improved the properties of the resulting PLA-based nanocomposite films.

Key words: Poly (lactic acid), food packaging, ZnO NPS,

Corresponding Email : **bencherikrebiha2023@gmail.com**

P-075

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Title: Homogenization of Heterogeneous Structures Using the Finite Element Method

Douaa KHELLADI [1], Amer MECELLEM[1], Imad ELFATMI[1], Sofiane BELHENINI[1]

Mechanical engineering, BELHADJ BOUCHAIB University, AIN TEMOUCHENT, ALGERIA

Abstract:

The miniaturization of electronic microcomponents is made possible by new integration techniques such as 3D integration. These new integration techniques require use of new materials in the form of stacked thin films. Finite element modeling of new generation microcomponents is complicated by the presence of several thin layers with complex geometries[1]. Most electronic systems continue to miniaturize and enhance functionality, and they are subject to constraints in the environment in which they are used. That's why the materials was developed with customisable properties to support the applied loads[2] and to minimize costs and save time. Therefore, several methods have been developed to estimate these properties but numerical periodic homogenisation is the most accurate.[3-4]. Homogenisation consists in replacing a heterogeneous medium by a homogeneous medium with the same behavior.[5]. The proposed method is applied to 3D model composed of three diffrent materials -Multi materials- was proposed by using finit element software, such as ABAQUS CAE, applied to it periodic boundary conditions in several phases -Tensile, Compression, Shear- This study focuses on the comparison between the homogenized behaviour and the a full model behaviour. An essential stage in the design and analysis of materials is estimating the effective elastic characteristics, and therfore, a good agreament is observed between those two, thus our approach is reliable.

Key words: Multi-Material, Thin films, Periodic Boundry condition, ABAQUS CAE, 3D modeling, Homogenization, Heterogeneous, Finite Element Modeling

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Deposition and Characterization of Nanostructured Copper Oxide (CuO) Thin Films using Sol-Gel Dip-Coating Technique

Redjouh Nour Elhouda, Redjouh Nour Elhouda; Belhamra Nedjette

Abstract

Copper oxide is a P-type semiconductor material that is black in color with a slight transparency. It is an interesting material for various applications due to the abundance of its components in nature, its good thermal stability and its structural and optical properties. This property allows it to be almost excellent in many applications such as catalysts, solar cells and batteries... In this work-in-progress, the solution was prepared by the Sol-Gel method and thin films of CuO were deposited on glass substrates by Dip Coating technique, this study focused on different film thicknesses by varying the frequent number of layers deposited. The effect of thickness on optical properties of CuO thin film were studied using the UV-VIS spectrometer to assess the transmission and energy gap and Structural properties using X-ray diffraction (XRD) in order to assess the Crystallite size.

keywords: Sol-Gel, Dip-Coating, Copper Oxide, Thin films, DRX, UV-V.

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Magnetic and structural properties of nanostructured FeSn alloys elaborated via ball milling process

Abderahim ABADA[a], Abderrahmane YOUNES[b], and Rachid AMRAOUI[b]

[a]Laboratory of Aeronautic Science, Aeronautic Institute, University of Saad Dahlab Blida 1, Blida,
[b]Research Center in Industrial Technologies (CRTI) P.O. Box 64, Cheraga 16014 Algiers, Algeria.

Abstract: This study investigates the impact of milling time on the magnetic properties of nanostructured Fe–Sn alloys synthesized via a ball milling process. The structural properties, morphological features, and magnetic behavior of the resulting nanostructured materials were analyzed using various characterization techniques, including scanning electron microscopy, energy-dispersive spectroscopy, X-ray diffraction, and vibrating sample magnetometer. After subjecting the samples to a grinding time of 10 h, XRD analysis revealed the presence of characteristic peaks corresponding to FeSn phase. The average crystallite size ranged from 51 to 18 nm, while the lattice strain was measured between 0.184% and 0.259%. Interestingly, the grinding process led to an increase in coercivity, remanence magnetization, and squareness of the nanostructured FeSn samples, accompanied by a decrease in saturation magnetization.

Key words: Nanostructured FeSn, milling time, Structural properties and Magnetic properties

Corresponding Email: abada_75@yahoo.fr

References

[1] D. Multer, J.X. Yin, M.S. Hossain, X. Yang, B.C. Sales, H. Miao, M. Zahid Hasan, Imaging real-space flat band localization in kagome magnet FeSn. Commun. Mater. 4(1), 17 (2023)

[2] B. Fayyazi, K.P. Skokov, T. Faske, D.Y. Karpenkov, W. Donner, O. Gutfleisch, Bulk combinatorial analysis for searching new rare-earth free permanent magnets: Reactive crucible melting applied to the Fe-Sn binary system. Acta Mater. 141, 434–443 (2017)

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Effect Of The Absorbent Layers On The Performances OF The SiGe Thin-Films Solar Cell

BOUKAIS Meriem[a,b], B. DENNAI[b], A.OULD ABBAS[c]

[a]Higher School in Electrical and Energy Engineering of Oran, Algeria
[b]Research Unit of Materials and Renewable Energies (URMER), University Abou Bakr Belkaïd, B.P. 119, Tlemcen, Algeria
[c]Laboratory for the Development of Renewable Energies and their Applications in Saharan areas (LDREASA)

Abstract:

The effect of absorber layer thickness and doping in thin-films solar cells is determined. For this, the current–voltage measurements of solar cell devices were carried out at room temperature under radiation (AM1.5) using AMPS-1D simulator software. The absorber layer (SiGe) designs for thin-films solar cells based Cds/SiGe is studied to determine their electrical performances as a function of the absorber thickness and doping concentration. The first step in this simulation is to study the effect of absorber layer (SiGe) thickness (from 10µm to 30µm) by keeping its doping constant (NA= 1 x 10^{17} cm^{-3}). In the second step the doping is varied and the optimum thickness obtained previously is kept constant. The maximum conversion efficiency of 17.90 % is obtained for 25µm and 1x10^{18} cm^{-3} for the optimal thickness and doping concentration respectively.

Key words: Simulation, AMPS-1D, SiGe, Thin-films, solar cell, efficiency

Corresponding Email: boukais_meriem@esgee-oran.dz

References

[1] Stephen J. Fonash, A manual for AMPS-1D, [online] Available: http://ampsmodeling.org/latest.html#manual
[2] J. Raman, U. P. Singh, Energy Environ. Sci. 10, 1306 (2017).
[3] T. Atouani, B. Dennai, A. Nouri, Journal of Nanoelectronics and Optoelectronics 13(1), 1 (2018)

P-079

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Ab-initio calculations of structural ,electronic,optical and thermoelectric properties of a noval hybrid double perovskite Na_2LiMgH_6 compound for advanced energy storage system

Lemya AMRANI[a,b], Djillali BENSAID [a,c], Habib RACHED[a,d]

[a]Magnetic Materials Laboratory, Science Exact Faculty, Djillali Liabes University of Sidi Bel Abbes, Sidi Bel Abbes, Algeria
[b] Faculty of science and technology, BelHadj Bouchaib University, Ain Temouchent, Algeria
[c] Electrical Engineering Faculty, Djillali Liabes University of Sidi Bel Abbes, Sidi Bel Abbes, Algeria
[d] Department of Physics, Faculty of Exact Sciences and Informatics (FSEI), Hassiba Benbouali University of Chlef, Chlef, Algeria

Abstract:

This current study investigates structural, electronic, optical, and thermoelectric properties of hydrud perovskite compound and its potential application in energy conversion and storage energy in technologies. Our calculations carried out within the Linearized Augmented Plane Wave (FP-LAPW) [1]method. This particular method relies on the Density Functional Theory (DFT)[2]. To treat exchange and correlation terms we have chosen -Perdew-Burke-Ernzerhof (GGA-PBE) [3] as well as modified Beck-Johnson correction (mBJ-GGA) [4]and the hybrid function (HSE06) . The package of this method is implemented in the WIEN2K code [5].First of one, we calculated the lattice constant, and our results were in close to theoretical and experimental findings available data.The band structure shows a semiconducting behavior with an indirect band gap We have determined the optical absorption coefficient, revealing a notable absorption ($>10^4$ cm^{-1}) in the visible spectrum.The optical absorption results demonstrate the significant potential of our material for applications in photovoltaic, optoelectronic devices, and solar cells.Thermoelectric properties alloys us determining the Seebeck coefficient and figure of merits ZT were calculated utilizing the Boltz-TraP code[6].

Key words: Perovskite, FP-LAPW, DFT, GGA, HSE06, WIEN2K, BoltzTraP, Seebeck coefficient.

P-080

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Computational prediction of structural, electronic, elastic, optical and thermoelectric properties of YVReZ (Z =Al , Ga, In) Yttrium based quaternary Heusler alloys for optoelectronic and thermoelectric applications: A DFT study.

Abdelli Abdelbasset[a,b], Hebri Salem[c] , Benkhettou Nour-eddine[b]

[a] Department of physics, Faculty of science and technology, University of Ain Temouchent Belhadj Bouchaib, BP284, Ain Temouchent, 46000, Algeria.
[b] Magnetic Materials Laboratory(LMM),University of Sidi-Bel-Abbes ,Sidi-Bel-Abbes, Algeria.
[c] Department of Exact Sciences, High Teaching School of Oran, Algeria.

Abstract:

In this work, we conducted simulations to examine the various physical properties of equiatomic Yttrium based quaternary Heusler alloys, YVReZ (Z = Al, Ga, In), using first-principle calculations. These calculations were performed using Full-Potential Linearized Augmented Plane Waves (FP-LAPW) [1] based on density functional theory (DFT) as contained in the Wien2k code [2] using (GGA) [3] and the hybrid function (HSE06) [4] approximations.The YVReZ compound crystallizes in the LiMgPdSn–type FCC cubic crystal structure within the F-43m space group, with three different configurations of atomic arrangements. The most stable configuration is determined through volume optimization calculations within the crystal structure. These compounds are found to crystallize in type I non-magnetic phase. The electronic properties were analyzed by calculating the band structure as well as the density of states (DOS). These compounds were observed to exhibit semiconductor behavior with indirect band gaps. Regarding the optical properties, our compounds exhibit good light absorption in the visible range, making them potential candidates for photovoltaic cells and optoelectronic applications. Additionally, we evaluated

the thermoelectric parameters using Boltz-TraP code [5] .The obtained calculations affirm the promising application of these materials in energy conversion technologies.

Key words: Quaternary Heusler alloys, FP-LAPW, DFT, Wien2k, GGA, HSE06, Boltz-TraP code.

Corresponding Email:
abdelbasset.abdelli@univ-temouchent.edu.dz
salem.hebri@gmail.com
nordine_bt@yahoo.com

References

[1] P. Blaha, K. Schwarz, G.K.H. Madsen, D. Kvasnicka, J. Luitz, K. Schwarz (Ed.),, WIEN2K. An Augmented Plane Wave and Local Orbitals Program for Calculating Crystal Properties, Vienna University of Technology, Vienna, 2001.
[2] P. Blaha, K. Schwarz, G.K. Madsen, D. Kvasnicka, J. Luitz, An Augmented Plane Wave+ Local Orbitals Program for Calculating Crystal Properties, 2001.
[3] J.P. Perdew, K. Burke, M. Ernzerhof, Phys. Rev. Lett. 80 (1998) 891.
[4] J. Heyd, G.E. Scuseria, M. Ernzerhof, Hybrid functionals based on a screened Coulomb potential, J. Chem. Phys. 118 (2003) 8207, https://doi.org/10.1063/ 1.1564060.
[5] Georg K.H. Madsen, David J. Singh, Computer Physics Communications,175,67-71, 2006.

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Electronic and thermoelectric properties of Half-Heusler compound: Spin orbit coupling effect

Khedija Talbi, Youcef cherchab, mohamed Belmiloud
Université de Relizane, Bormadia Relizane 048000, Algeria.

Abstract

We investigate electronic structures and thermoelectric properties of new Half Heusler RbLaGe. The structural and dynamic stabilities of RbLaGe are proven and the direct relationship between the SOC effect and phonon calculations is shown. The spin-orbit coupling (SOC) has strong influence on the valence band of RbLaGe compound with a split of about 0.13eV at the highest point and along [001] magnetization. Additionally, the spin-orbit coupling (SOC) decreases slightly the band gap of this material. Our obtained results show that RbLaGe has high thermopower resulting from the favorable features of its band structure. The SOC effect on the thermoelectric properties of RbLaGe compound, including Seebeck coefficient, electrical conductivity, electronic thermal conductivity and power factor. The power factor increases with increasing temperature and its maximum value at 800 K is found between 5.9 10 × 11 (W/mK2 s) and 6.3 10 × 11 (W/mK2 s.

Keywords: FP-LAPW, Half-Heusler , phonon calculations, Electronic properties,Thermoelectric properties , Spin-orbit coupling effect

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Effect of Magnesium on the dielectric properties of an alloy (Al-3%Mg) alloy for humidity sensor applications

Hakima Aidrous *1, Imane Chikhaoui2, Nouara Lamrani2, Ahcène Chaouchi2.
1Département de Chimie, Faculté des Sciences, Univ. UMMTO, Tizi Ouzou, Algéria
2Laboratoire de Chimie Appliquée et Génie Chimique, Univ. UMMTO, Tizi Ouzou, Algéria

Abstract

Light alloys, aluminium and magnesium, offer a wide range of applications thanks to their good compromise (density, mechanical properties). In addition to their low density, aluminium alloys have good corrosion resistance thanks to the natural protective oxide layer that forms spontaneously on their surfaces, ease of forming and good electrical conductivity. The main objective of this work is to develop and study the application of pure aluminium sinter and the alloy (Al-3%Mg) in the design of humidity sensors. The samples obtained after sintering in a vacuum for 5 hours at 550°C are characterised structurally by X-ray diffraction, and microstructurally by scanning electron microscope, and by density measurement using the Archimedes push method. The electrical properties of the sensors produced were studied using complex impedance spectroscopy (CIS). The humidity detection properties of the two elements (pure Al and the alloy (Al-3%Mg)) were studied at a frequency of 100 Hz and over the relative humidity (RH) range from 12 to 87% at room temperature. In terms of sensitivity, the sensors showed an increase in sensitivity throughout the humidity range studied. It was also noted that the addition of magnesium to the aluminium matrix considerably improved the response of the sensors. The maximum hysteresis of the alloy is 23.32% at 100 Hz. The complex impedance spectrum has enabled us to understand the behaviour of water molecules on the surface of the sensors through the adsorption mechanism. The results of this study showed that the addition of magnesium offers promising characteristics as a moisture-sensitive material.

Keywords: humidity sensor, alloy, impedance, sensitivity, hysteresis

P-083

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Impact of Convergent Angle Variations on Rocket Nozzle Performance parameters

Nabila ALILI[a,*], Mohammed Amine DJEFFAL[b] , Khacem KADDOURI[a], Mokadem SALEM[a], ,and Ali BENOUAR [c]

[a] Mechanical Engineering Department, Djillali Liabes University, Laboratory of Physical Mechanics of Materials (LMPM), City Larbi Ben Mhidi, P.O. Box 89, 22000 Sidi Bel Abbes, Algeria.
[b] Mechanical Engineering Department, Djillali Liabes University, Laboratory of Materials and Reactive Systems (LMSR), City Larbi Ben Mhidi, P.O. Box 89, 22000 Sidi Bel Abbes, Algeria.
[c] Higher School of Electrical and Energy Engineering ESGEE, Laboratory of complex systems (LCS), Oran, Algeria

Abstract:

Unveiling the optimal dance between convergent angle and exhaust performance in rocket engine nozzles, a comprehensive numerical analysis waltzed through a spectrum of angles (20°-45°). This intricate exploration, employing the Realizable k-ε turbulence model, meticulously measured the impact on key parameters like velocity coefficient (Cv), adiabatic efficiency, and gross thrust coefficient (Cfg). Not stopping at geometry, the analysis delved deeper, investigating the influence of nozzle pressure ratio (NPR) on these crucial metrics. This multi-dimensional journey led to the discovery of the sweet spot at 35° convergent angle, maximizing thrust generation efficiency.

Key words: Convergent angle, Realizable k-ε turbulence model, Velocity coefficient (Cv), thrust coefficient (Cf), Nozzle pressure ratio (NPR)

* Corresponding author. Tel: +213 673410525
E-mail address: alili.16nabila@gmail.com*, nabila.alili@univ-sba.dz

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

All Optical 1D Ternary Photonic Crystal Biosensor for Detection of Cancerous Brain Cells

Iman OUAHAB, Samia DRIZ, Benattou FASSI

Telecommunications and Digital Signal Laboratory, University Djillali Liabes, Algeria

Abstract:

In this work, an all-optical biosensor based on 1D ternary photonic crystal was created for detection of tumor 's Brain cells. A defect was infiltering in structure to create a mode defect. The Transfer Matrix Method was exploited for modelling the transmittance profile and the mode defect was monitored.

The proposed all optical biosensor is very sensitive, offers a simplicity in design, and operates at a nano-scale size. These characteristics cover the way for a viable and practical approach to diagnosing cancerous cells.

Key words:

Ternary photonic crystal, Biosensor, Sensitivity, Mode Defect, Cancerous Brain cells.

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Effect of Magnesium on the dielectric properties of an alloy (Al-3%Mg) alloy for humidity sensor applications

M.Dine.Elhannani[1] , M.Ameri [1] .

[1.] University Djillali Liabbes Sidi Bel Abbes . Physico-Chemiistry Laboratory of Advanced Materials

Abstract

Using first-principle density functional calculations, the structural, electronic and magnetic properties of cubic perovskite LaFeO3 were studied by means of the full potential linear muffin-tin orbital method. Calculations were performed within the local spin density approximation (LSDA) to the exchange correlation potential. The magnetic phase stability was determined from the total energy calculations for both ferromagnetic (FM) and non-magnetic (NM) phases. Our calculations show that the magnetic phase is more stable than the non-magnetic phase. To our knowledge the elastic constants of this compound have not yet been measured or calculated, hence our results serve as a first quantitative theoretical prediction for future study. Additionally, the band structure, the density of state and the magnetic moments were analyzed.

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Investigation Of Re(I)-Tricarbonyl 1-2-4 Triazol Complexes By DFT Method

BOUKERTOUTA Ghadir[a], SERIDI Achour[a].

[a] Laboratory of physical chemistry, University 8 May Guelma, Algeria.

Abstract:

Many organometallic complexes exhibit considerable cytotoxicity towards cancer cells in recent decades, and these complexes are being used in explored anti-cancer therapy candidates. Of the different metal ions being investigated, complexes of rhenium are among the most promising candidates for therapeutic applications. Rhenium complexes have several advantages over conventional organic drugs currently used to treat cancer.

In this study, stable complex between a 1,2,4 triazole derivative and tricarbonyl rhenium is studied theoretically, using Gaussian 09 and the DFT method. The free ligand is optimized with the hybrid function B3LYP and 6-31G(d) basis set and the complex with the mix bases set of B3LYP-LanL2DZ/6-31G(d). Different parameters were calculated including frontier molecular orbitals energies, reactivity indexes and molecular electrostatic potential allowed us to locate the sites of nucleophilic and electrophilic attack. Further data such as vibrational frequencies and UV-VIS spectra of the free ligand and the complex.

Key words: Rhenium complex, DFT, HOMO, LUMO.

Corresponding Email: Boukertouta.ghadir@univ-guelma.dz / boukertouta24ghadir@gmail.com .

P-087

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Numerical Investigation of Aspect Ratio Impact on Regenerative Cooling Heat Transfer in Liquid Propellant Rocket Engines

Mohammed Amine DJEFFAL[a*], Nabila ALILI[b], Nabil BENAMARA[a], Abdelkader LAHCENE[a], Khacem KADDOURI[b], Abdelkader BOULENOUAR[a]

[a]Laboratory of Materials and Reactive Systems (LMSR), Mechanical Engineering Department, Djillali Liabes University, Sidi Bel Abbes, Algeria.
[b]Laboratory of Physical Mechanics of Materials (LMPM), Mechanical Engineering Department, Djillali Liabes University, Sidi Bel Abbes, Algeria.

Abstract:

This study investigates heat transfer in regeneratively cooled liquid propellant rocket engines (LPREs) using methane as the coolant. Through numerical simulations, we analyze the influence of the aspect ratio of three rectangular channels, on heat transfer performance with asymmetric bottom wall heating. The results reveal that "Rec-3", a rectangular channel with the highest aspect ratio (greater than 1), exhibits the most significant reduction in bottom wall temperature Twg compared to the two other configurations. However, this improvement comes at the cost of increased pressure losses. Conversely, "Rec-1" (aspect ratio less than 1) showcases the best performance in terms of top wall temperature Twa, a crucial result for next-generation engines employing composite overwrapping.

Key words: Regenerative cooling, Supercritical Methane, Heat transfer, Liquid propellant rocket engines, Rectangular channels, Aspect ratio

[*] Corresponding author. Tel: +213 549377813
E-mail address djeffalmohammed66@gmail.com*, mohammed.djeffal@univ-sba.dz

P-088

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Investigation of structural, mechanical, electronic and thermodynamic properties of $YLuNi_2Sb_2$ double half Heusler: FP-LAPW Method

Amel SLAMANI[a], Friha Khelfaoui[b]

[a]Department of Physics, Faculty of Science and Technology, University of Relizane,48000, Algeria
[b]Department of Physics, Faculty of Sciences, university of Moulay Tahar Saida, 20000, Algeria.

Abstract:

The theoretical calculations of structural, mechanical, electronic and thermodynamic properties of new double half Heusler $YLuNi_2Sb_2$ have been investigated employing FP-LAPW method. We have explored the mechanical stability following Born criteria additionally the compound is brittle and anisotropic, our alloy is semiconductor in tetragonal structure with indirect band gap. We have also elucidated the thermodynamic properties with quasi harmonic Debey approximation. The effect of temperature and pressure on bulk modulus, thermal expansion coefficient, heat capacity and Debey temperature are presented.

Key words: FP-LAPW, double half Heusler, Born criteria, Debey temperature.

Corresponding Email:

References

[1] slmnamel@yahoo.fr

P-089

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Title: Revealing half metallicity of new full-Heusler compound

GUERMIT Youcef[a], K. HOCINE[a], M. Drief[b], S.Mesbah[a], N. Benkhettou[c], D. Rached[c]

[a] Relizane university, Algeria
[b] Bouira university, Algeria
[c] Sidi belabess university, Algeria

Abstract:

Half metallic (HM) materials have attracted a lot of interest due to their potential applications such as magnetic sensors [1-2]. Researchers are interested in employing Heusler compounds in spintronics devices because of their ferromagnet features, which include a gap in one of the spin directions at the Fermi energy EF and 100% spin polarization at the Fermi level [3]. The aim of this study is to calculate using Density Functional Theory (DFT of, the electronic structure, magnetic, and elastic properties of the recently discovered full-Heusler compound Ir_2CoSn are investigated. The Cu_2MnAl and Hg_2CuTi prototype structures are compared for ferromagnetic (FM) and non-magnetic (NM) states. It has been discovered that in these two types of structures, the ferromagnetic state in the Cu_2MnAl structure is energetically more stable than the nonmagnetic state. Then the total density of states and band structures were plotted using GGA and mBJ methods, the spin-polarized calculations show that the spin-up electrons of Ir_2CoSn compound have metallic nature, but the spin-down electrons have semiconducting behavior with 0.23 eV energy gap around the Fermi level. The calculated Cauchy pressure and Poisson's ratio indicated that Ir2CoSn compound is a ductile material. Ir_2CoSn compound is a half-metallic ferromagnetic (HMF) and it has 2.99 μB magnetic moment. This study will theoretically lead to experimental works in the spintronic field and its applications.

Key words: Full-Heusler, DFT, half-metallic, spintronic.

Corresponding Email: gyoucef75@gmail.com

References

[1] S.A. Wolf, D.D. Awschalom, R.A. Buhrman, J.M. Daughton, S. von Molnar, M.L. Roukes, A.Y. Chtchelkanova, D.M. Treger, Science 294 (2001) 1488.
[2] I. Zutic, J. Fabian, S. Das Sarma, Spintronics: fundamentals and applications, Rev. Mod. Phys. 76 (2004) 323.
[3] E. Şaşıoğlu, L.M. Sandratskii, P. Bruno, I Galanakis, Exchange interactions and temperature dependence of magnetization in half-metallic Heusler alloys, Phys.Rev. B. 14 (18) (2005) 18441572.

P-090

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

A computation exploration of physics properties of new iradium based ful-Heusler

Kamel. HOCINE[a], Y. GUERMIT_[a], M. Drief[b], S.Mesbah[a], M. Rabeh[c], D. Rached[c]

[a] Relizane university, Algeria
[b] Bouira university, Algeria
[c] Sidi belabess university, Algeria

Abstract:

Due to its prospective uses in applications like magnetic sensors, half metallic (HM) materials have garnered a lot of attention [1-2]. Because of their ferromagnet characteristics, which include 100% spin polarization at the Fermi level and a gap in one of the spin directions at the Fermi energy EF, researchers are interested in using Heusler compounds in spintronics devices [3]. In this work, the electronic structure, magnetic, and elastic characteristics of the recently discovered full-Heusler compound Ir_2MnSn are calculated using Density Functional Theory (DFT). The normal and inverse prototype structures are compared for ferromagnetic (FM) and non-magnetic (NM) states. It has been discovered that in these two types of structures, the ferromagnetic state in the Cu_2MnAl structure is energetically more stable than the nonmagnetic state. Then the total density of states and band structures were plotted using GGA and mBJ methods, the spin-polarized calculations show that the spin-up electrons of Ir_2MnSn compound have metallic nature, but the spin-down electrons have semiconducting behavior with 0.12 eV energy gap around the Fermi level. The calculated Cauchy pressure and Poisson's ratio indicated that Ir_2MnSn compound is a ductile material. Ir_2MnSn compound is a half-metallic ferromagnetic (HMF) and it has 5μB magnetic moment. This study will theoretically lead to experimental works in the spintronic field and its applications.

Key words: Full-Heusler, mBJ, half-metallic, spintronic.

Corresponding Email: hocine_kamel@yahoo.com

References

[1] I. Zutic, J. Fabian, S. Das Sarma, Spintronics: fundamentals and applications, Rev. Mod. Phys. 76 (2004) 323.
[2] R.A. de Groot, F.M. Mueller, P.G. van Engen, K.H.J. Buschow, New class of materials: half-metallic ferromagnets, Phys. Rev. Lett. 50 (1983) 2024.
[3] C.M. Fang, G.A. de Wijs, R.A. de Groot, Spin polarization in half-metals, J. Appl. Phys. 91 (2002) 10.

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Effects of oxygen flow during the annealing process of doped emitters in n-type monocrystalline silicon wafers.

LABDELLI B[#1], BOUCHEHAM A[1], BENHARRAT L[1], DJELLOUL A[1], BEKHEDDA K[1] DJEMA O[1], MAREF A[1], NASRAOUI C[1] and MAZARI H[2]

[1] *Research Center in Semiconductor Technology for the Energetic (CRTSE) 2, Bd Frantz Fanon, B.P. 140,7M, Alger-, Algeria;*

[2] *Applied Microelectronics Laboratory, Department of Electronics, Sidi Bel Abbes University, B.P. 89, 22000 Algeria;*

Abstract:

We demonstrate that the concentration of electrically inactive phosphors of the emitter has a significant impact on the development behavior of a SiO_2 layer after the annealing process on CZ monocrystalline silicon wafers. Boron-oxygen defect has an energy level close to the mid-gap in p-type solar cells; a grown-in point defect creates a complex of interstitial oxygen dimer and substitutional boron [1]. For this reason, solar-grade n-type Czochralski (CZ) c-Si wafers (4-inch) with ⟨100⟩ crystal orientation, 1–3 Ω cm resistivity, and 360 µm thickness are used for this study. Two structures, n-900 and n-850, were fabricated at 900 °C and 850°C for the same deposition time of 20 min in the LYDOP type with $POCl_3$ diffusion furnace and the same parameters (gas flow) in order to create phosphorus-doped n+ front surface field (FSF) in N-type PERT (passivated emitter rear totally diffused) silicon solar cells promise high and stabilized conversion efficiencies [2.3]. The annealing process adjusts the oxygen flow from 0 to 4 Slm (Standard liter per minute) after phosphosilicate glass (PSG) removal using hydrofluoric acid (HF). We can conclude that the quality of passivation depends greatly on temperature. In fact, when the volume of oxygen flow increased throughout the annealing process, the effective lifetime increased dramatically to a maximum value of over 180

microseconds at a temperature range of 850°C. We discovered that the volume of oxygen flow necessary for annealing is 2 SLM at 900°C.

Key words: Cz-Si n type, $POCl_3$, Annealing process.

Corresponding Email: labdeliB@crtse.dz , boutaleb200574@yahoo.fr

---

References

[1] K. Bothe, R. Sinton, J. Schmidt (2005) Fundamental boron-oxygen-related carrier lifetime limit in mono- and multicrystalline silicon. Prog Photovolt Res Appl 287-296.

[2] S. Singh et al., "Laser doping from PSG for selective FSF of screen printed rear-junction n-PERT cells," in Proc. 35th Eur. Photovolt. Sol. Energy Conf. Exhib., Brussel, Belgium, 2018, pp. 580–583

[3] A. El Amrani1 et al, Silicon 2020. https://doi.org/10.1007/s12633-020-00809-3

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Title: **Study of the Mechanical Behavior of a Standardized Arc-shaped Specimen in PVC**

Rebehi Kheira[a,1], Abdel-Nour Zaim[a,2], Ali Boudjlall Moulai1[b,3], El Bahri Ould Chikh[a,4],

[a]LSTE Laboratory, University of Mascara, BP 305 Route de Mamounia Mascara, Algeria.
[b]Department of Mechanical Engineering, University of Relizane, Algeria.
[1] rebehikheira@gmail.com [2]za.abdelnour@yahoo.fr, [3]djallelmoulay@yahoo.fr, [4]chikhb@yahoo.com,

Abstract:

Our work consists of conducting a numerical modeling study on a slender PVC arc-shaped specimen with an internal notch (defect) within the arc, subjected to uniaxial loading at different ratios (a/w). The numerical results obtained allowed us to analyze the influence of this ratio (a/w) on the plastic deformations that occur at the notch. To carry out this work, we relied on the ASTM E399-90 (1997) standard to obtain a standardized specimen and to determine stress concentrations at crack points.Through the obtained results, we observed that plastic deformation confined at the crack tip propagates along the ligament as the ratio (a/w) increases. Additionally, we noticed that the ratio a/w=0.55 yields insignificant results, suggesting that this ratio may represent a critical value for defects in polymer conduits.

Key words: plastic deformation ; Polyvinyl Chloride , arc-shaped specimens, ratios (a/w)

P-093

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Synthesis, characterization and bio activities of poly(1-2(Dihydroxyethyl)-3-vinylimidazolium) (poly (ionic liquids))

Bassou Djilali**, Chaker Yassine*, Abdelkader Benabdellah*.

**Laboratoire de chimie organique physique et macromoléculaire, Université de Sidi Belabbes
Bjilali@yahoo.com
*Laboratoire de Synthèse et Catalyse LSCT, Université de Tiaret, BP 78 RP 14000 Tiaret, Algeria chaker.
yassine@univ-tissensilt.dz
abdelkader.benabdelah@univ-tiaret.dz

Abstract

he analogous molecule, 1-2 Dihydroxyethyl-3-vinylimidazolium chloride [DEtOHVIM+] [Cl-], was created chemically when 3-Chloro-1,2-propanediol and 1-vinylimidazol were used as precursors. In the following step, [DEtOHVIM+][Cl-] was treated with 2,2-azobisisobutyronitril (AIBN) to produce poly[DEtOHVIM+][Cl-], which is a poly1-2(Dihydroxyethyl)-3-vinylimidazolium chloride. Finally. As a first step in spectroscopic characterization, 1H-NMR and 13C-NMR were used to determine the structure of these molecules. In order to learn more about the structure and vibrational behavior of these compounds, Fourier Transform-Infrared-Attenuated Total Reflectance and Fourier Transform Raman spectroscopy measurements were made in the spectral ranges 600–4000 cm-1 and 0–3500 cm-1, respectively. Additionally, three types of thermal analysis—thermogravimetric analysis (TGA), differential thermal analysis (DTG), and differential scanning calorimetry (DSC)—are used to comprehend the thermal stability of these substances. The poly1-2(Dihydroxyethyl)-3-vinylimidazolium chloride shows important antioxidant properties

Keywords: Vinylimidazolium chloride, DTG, DSC , AIBN

P-094

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Wave propagation response of double – walled carbon nanotubes

Leila Djazia Benmansour[a,b], Fouad Bourada[c], Houari Heireche[b]

[a] Université des Sciences et de la Technologie Houari Boumediene, faculté de physique, Alger, Algérie
[b] Laboratoire de Modélisation et Simulation Multi-échelle, Université Sidi Bel Abbes, Algérie
[c] Laboratoire des Matériaux et Hydrologie, Université Sidi Bel Abbes, Algérie

Abstract:

This investigation studies the vibrational characteristics of double – walled carbon nanotubes (DWNTs) with initial stress [1] using a nonlocal Euler – Bernoulli beam model. Both the effect of initial stress and the effect of small length scale are discussed. The effect of van der Waals forces [2] is incorporated in the formulation. The corresponding resonant vibrational characteristics are presented, which are shown to be very different from those predicted by classical elasticity theory when nonlocal effects are significant. The influence of initial stress in carbon nanotubes on their flexural vibration modes is dependent on the tension or compression forms of the initial stress.

Key words: DWNTs, Euler-Bernouli beam model, Nonlocal effect.

Corresponding Email: djaziabmsr@gmail.com

References

[1] Zhang Y, Liu G and Han X "Transverse vibrations of double-walled carbon nanotubes under compressive axial load" Phys. Lett. A 340 (2005), 258-266.

[2] B. Reulet *et al*, Phys. Rev. Lett. **85**, 2829 (2000).

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Optimization of experimental parameters for the electrodeposition of Cobalt-Molybdenum metal layers on a silicon substrat

Z. Fekih[(a)], N. Gabouze[(b)], S. Sam[(b)], N.Ghellai[(c)] and N. E. Chabanne-Sari[(c)]

(a). Materials physics and apllications Laboratory, Université B. B. AinTemouchent, Algeria
(b). C. R. T. S. E, 2Bd Frantz-Fanon, B.P .140, 7merveilles Algiers, Algeria,
(c). U.R.M.E.R University Abou –Baker Belkaid B.p: 119 TLEMCEN 13000 Algeria

Abstract:

Cobalt-molybdenum alloy is electrochemically deposited on a heavily doped n-type silicon (Si-n+) substrate. However, several parameters influence the characteristics of the deposited film. In this work we studied the influence of the concentration of Molybdenum and the PH of the solution. CoMo films deposited from solutions containing different concentrations of Mo on the one hand and different PH values on the other were characterised by X-ray diffraction (XRD), energy dispersive X-ray spectroscopy (EDS) and scanning electron microscopy (SEM).

The films obtained from solutions with low concentrations of Mo and low acidity of the solution show good adhesion with the substrate, crystallinity of the deposit with a remarkable peak of the CoMo alloy and contain less Molybdenum oxide[1].

Key words: Thin films, Metal alloys, Electrodeposition.

Corresponding Email: zakia.fekih@univ-temouchent.edu.dz

References

[1] . Z. FEKIH «Electrodéposition des métaux (Fe, Ni, Mo, Co…) sur silicium et silicium poreux » Thèse de Doctorat, Département de physique, U.R.M.E.R, université de Tlemcen, Décembre 2003.

P-096

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Investigating Thin Films of Lead Sulfide (CdS): Production, Analysis, and Theoretical Perspectives for Implementing Biological Detection Devices.

Kheira Ouari*, [1], Kheira Ameur[2], Halima Mazari[2], and Abdelkader Nakrela[2]

[1] Department of Automatics, University Djillali Liabes of Sidi Bel Abbes, 22000 Sidi Bel Abbes, Algeria
[2]Department of Electronics, University Djillali Liabes of Sidi Bel Abbes, 22000 Sidi Bel Abbes, Algeria

Abstract:
The current manuscript presents a comprehensive examination of thin films comprising cadmium sulfide (CdS) [1] through a combination of theoretical and experimental methodologies. The structural and morphological characteristics of these films, produced utilizing the spray pyrolysis technique, were assessed using X-ray diffraction (XRD) and scanning electron microscopy (SEM). An investigation into the reflectance and transmittance spectra in the [1.5-3.5] eV range of a thin CdS film was conducted. Theoretical calculations were performed using the first principles full potential linearized augmented plane wave (FP-LAPW) method. The outcomes of this analysis indicate that the CdS film under scrutiny possesses a polycrystalline nature[2] and displays a wurtzite structure. The SEM imagery demonstrates a flat configuration with dimensions ranging from 480 to 930 nm. Data from energy dispersive spectroscopy (EDS) indicate a high degree of crystallinity, while the film surface exhibits a rough texture and a compact morphology. CdS acts as a semiconductor with a direct optical band gap located at the Γ point of the Brillouin zone (BZ) with respect to its electrical properties. The density of states on either side of the band gap is predominantly characterized by s-p attributes. The ionic characteristics of CdS can be ascribed to charge transfer processes. A significant level of concordance is observed between the experimental findings and the theoretical projections. Our current research endeavors are focused on investigating biosensors and their diverse range of uses.

Key words: FP-LAPW method, Spray pyrolysis technique, EDS, cadmium sulfide

Corresponding Email:

Ouari_K@yahoo.fr

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Structural, electronic, elastic and optical properties of Sc based equiatomic quaternary Heusler compounds

Miloudi Mohamed Esseddik[1,2], Salem Hebri[3], Benkhattou Noredinne[2]

[1] Department of physics, Faculty of science and technology, University of Ain Temouchent Belhadj Bouchaib, BP284, Ain Temouchent, 46000, Algeria.
[2] Magnetic Materials Laboratory(LMM),University of Sidi-Bel-Abbes ,Sidi-Bel-Abbes, Algeria
[3] Department of Exact Sciences, High Teaching School of Oran, Algeria.

Abstract:

This investigation reports the structural, electronic, optical and elastic properties of Sc-based quaternary Heusler alloy ScXTcGa (X=Nb, Ta or V) by density functional theory. For accurate determination of electronic structures, calculations were conducted using the hybrid HSE06 functional, yielding band gap values that closely match experimental findings. The energy band gaps of the quaternary Heusler semiconductors range from 1.30 to 1.57 eV, indicating their potential suitability for a wide range of applications. The optical analyses are fully integrated into this study, offering comprehensive insights into their optical properties. Additionally, elastic constants are computed to confirm the mechanical and dynamical stabilities of these alloys.

Key words: Quaternary Heusler -hybrid functional -Electronic band structure -Absorption coefficient

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Classical and ultrasonic preparation of new copper based nanocomposites: Application in the antimicrobial activity

Amel ILES[1], Farouk ZAOUI[2,3] , Khadra SOBRIK[3],Saadia BELKIOUR[3] , Bouchra ELHADJ DAOUADJI[3], Boumediene BOUNACEUR[3] , Fouad LEBSIR[3]

[1] Laboratoire de Synthese Organique Appliquée (LSOA), Faculté des sciences exactes et appliquées, Université Oran1 Ahmed Ben Bella, 31000 Oran, Algeria
[2]Centre Universitaire ElCherif Bouchoucha -Aflou-, B.P 306, Aflou, Laghouat, Algeria
[3]Laboratoire de Chimie Physique Macromoleculaire L.C.P.M, Universite Oran1 Ahmed Ben Bella, El-Menaouer, B.P 1524, 31000 Oran, Algeria

Abstract:

Water is one of the most precious natural resources on the planet, for all living creatures; therefore, its pollution is a very serious topic that worries several research groups.
Despite the fact that pollution causes a lot of disaster for living creatures, it, unfortunately, helps to fortify and reinforce the resistance of microorganisms that cannot be eliminated by the same techniques used to remove organic pollutants.
A new dendrimer based on citric acid and sebacoyl chloride was synthesized by Steglich esterification. The obtained dendrimer was used as a matrix for the dispersion of copper nanoparticles using classical and ultrasound methods. The obtained nanocomposites were tested against two Gram-positive pathogenic bacteria (Bacillus cereus and Staphylococcus aureus), two Gram negative (Escherichia coli and Pseudomonas aeruginosa) and against fungus species (C. albicans).
The comparative study between both methods has demonstrated that the materials synthesized by the classical method have all given a better antimicrobial activity, than those by ultrasound.
Key words: antimicrobials, citric acid dendrimers, copper nanoparticles.

Corresponding Email: ilesamel261@gmail.com

References

F. Zaoui, B. Elhadj Daouadji, M. Beldjilali, M. Hachemaoui, F. Z. Sebba, A. Mokhtar, B. Boukoussa.Classical and ultrasonic preparation of new dendrimer–Copper nanocomposites: Application in the catalytic reduction, antioxidant, and antimicrobial activities. Applied Organometallic Chemistry (2023) DOI: 10.1002/aoc.7099

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

moleculary imprinted films for bisphénol A retention

Aymen M. ZEHOUANI1[a], L. BEDJAOUI-ALACHAHE[a]

[a]Laboratory of Research on Macromolecules (LRM), Faculty of Sciences, University of Abou Bekr Belkaid, 13000, Tlemcen, Algeria

Abstract

This study details the synthesis and characterization of molecularly imprinted acrylate films created using a sandwich method with isobornyl acrylate (IBOA) and acrylic acid as monomers, targeting the selective retention of bisphenol A (BPA). Our primary focus was on optimizing the extraction process of the BPA template after polymerization and assessing the retention capacity of the films at a set concentration. To evaluate the structural integrity and functional properties of the imprinted films, we employed both spectral and thermal analysis techniques. Spectral methods, including UV-Vis and FTIR spectroscopy, were used to confirm the successful extraction of BPA and to investigate the presence of functional groups responsible for the selective interaction with BPA. Thermal methods, such as differential scanning calorimetry (DSC) and thermogravimetric analysis (TGA), provided insights into the thermal stability and decomposition patterns of the polymerThe results from these characterization methods demonstrated that the films possess specific molecular recognition sites for BPA with excellent thermal stability, making them suitable for potential use in environmental applications to remove BPA from water systems effectively.

Keywords: Bisphenol Aacrylic, Polymer , retention

Corresponding Email: aymen_zehouani@yahoo.com

References

P-100

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Title: Enhancement in Photocatalytic Properties of Sn-Doped La_2O_3 Nanostructures

Nesrine BLAHA[b], Younes MOUCHAAL[a,b], Lamia BARKAT[b] , Abdelbacet KHELIL[b]

[a] Faculty of Exact Sciences, Mustapha Stambouli University of MASCARA, Algeria.

[b] LPCMME Laboratory, Faculty of Exact and Applied Sciences, Oran 1 Ahmed Ben Bella University, Algeria.

Abstract:

Although the photo-catalytic degradation of dyes and other pollutants in air and wastewater by metal oxides is widely recognized as highly efficient, the cost associated with UV radiation usage remains a significant barrier to its large-scale applications [1]. One potential solution to transition from UV activation energy to the visible spectral range (Vis) could involve employing hetero-structures with a reduced band gap [2].

This project aims to investigate the visible light photo-catalytic performance of hetero-structured oxide thin films, focusing on enhancements facilitated by metal doping. The research will also explore the effects of varying dopant concentrations and annealing on the optical and electrical properties of La_2O_3.

After these structures were optimized, they were tested in the elimination of methylene blue dyes, under Vis radiation and under simulated solar radiation.

All the samples under investigation were used for photo degradation with Methylene Blue (MB). In less than 30 min of visible light irradiation, Sn doped La_2O_3 samples reached 99% of MB degradation activity.

This study showed that thin films can be used as a cost-effective material for the depollution of polluting organic compounds with modular physical properties.

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Study of the antimicrobial effectiveness for spinel ferrite nanoparticles of manganese-cobalt doped with cerium

Tahraoui Tarek [a], Debboub Salima [b], Chidouh Amina [c], Cheribot Cherif Maroua [c], Barhouchi Badra [d]

[a] L3M Laboratory, National Higher School of Technology and Engineering - ENSTI Annaba, Algeria

[b] Department of Physics, Chadli Bendjedid University, El Tarf, Algeria

[c] Department of natural sciences, Higher Normal School of Technological Education of Skikda,Algeria

[d] Pharmaceutical Sciences Research Center (CRSP), Constantine, Algeria

Abstract:

Currently, copious studies focus on nanoparticles as an alternative for new antimicrobial medecines.

The main scope of this research is to assess the antimicrobial effectiveness for spinel ferrite nanoparticles of manganese-cobalt that is doped with cerium synthesized with the coprecipitation method ($Mn_{0.5}Co_{0.5}Ce_{0.1}Fe_{1.9}O_4$NPs).

Nanoparticles of $Mn_{0.5}Co_{0.5}Ce_{0.1}Fe_{1.9}O_4$ have been analyzed with Fourier transform infrared spectroscopy (FTIR), X-ray scattering (XRD) and scanning electron microscopy (SEM) combined with X-ray spectroscopy energy dispersive method (EDS) to identify both the structural and morphological properties and chemical composition of these nanoparticles.

The antimicrobial activity of the synthesized nanoparticles is qualitatively evaluated using an agar diffusion disk, followed by determination of minimum inhibitory content (MICs).

The results show that the synthesized $Mn_{0.5}Co_{0.5}Ce_{0.1}Fe_{1.9}O_4$ nanoparticles have an outstanding antimicrobial activity against selected microbial strains afterward could be exploited for biomedical purposes.

Key words: nanoparticles, spinel ferrites, coprecipitation, antibacterial activity.

Corresponding Email: debboub-salima@univ-eltarf.dz

P-102

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Comparative study of ground-motions predicted using stochastic and neuro-fuzzy models

Zouheyr DIF [a,b], Boumédiène DERRAS [a,c]

[a] RISAM Research Laboratory, University of Abou Bekr Belkaid, Tlemcen, Algeria
[b] Department of Hydraulic and Civil Engineering, Science and Technology Institute, University Centre of Maghnia, Tlemcen, Algeria
[c] Department of Civil Engineering and Hydraulic, University of Saida, Saida, Algeria

Abstract:

In this study, 5% damped ground-motions represented by Pseudo Spectral Acceleration (PSA) at 0.1 s and 1.0 s, Peak Ground Acceleration (PGA) and Peak Ground Velocity (PGV) are computed using two different methods. The first one is based on the physics of earthquakes that called stochastic method, and the second method is based on the Adaptive Neuro Fuzzy Inference System (ANFIS) that used in this study a large subset of the Next Generation Attenuation (NGA)-West 2 reel ground motion database. The dataset distribution illustrated represents 4899 records from 1745 sites and 100 earthquakes. The input variables are: the moment magnitude (M_w) with a range between 4.5 and 6.5, the hypocentral distance (R_{hyp}) and the average shear-wave velocity over a subsurface depth of 30 m (V_{S30}). Ground-motions from the two models are compared, the results show convergences of the spectra, that are able to reproduce the NGA-West 2 observed data.

Key words: ANFIS, Database, Ground-Motion, Magnitude, NGA-West 2, Prediction.

Corresponding Email: difzouheyr@yahoo.com

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Towards New Horizons: Silver Nanocomposites Based on Smart PVA-g-Grafted Copolymers (PAA co PS)

[a , b] Radja Megherbi , [b] Fatima Bekkar , [b] Benzait Saadia Nawel, [b] Boutchiche Abdellah [1] , [a,b] Noureddine Bettahar

[a] Laboratory of Chemistry of Inorganic Materials and Applications (LCMIA),
[b] Department of Materials Engineering, Faculty of Chemistry, University of Science and Technology of Oran "Mohamed Boudiaf" (USTO.MB), BP 1505 El Menaouer , Oran 31000 , Algeria

Abstract

he analogous molecule, 1-2 Dihydroxyethyl-3-vinylimidazolium chloride [DEtOHVIM+] [Cl-], was created chemically when 3-Chloro-1,2-propanediol and 1-vinylimidazol were used as precursors. In the following step, [DEtOHVIM+][Cl-] was treated with 2,2-azobisisobutyronitril (AIBN) to produce poly[DEtOHVIM+][Cl-], which is a poly1-2(Dihydroxyethyl)-3-vinylimidazolium chloride. Finally. As a first step in spectroscopic characterization, 1H-NMR and 13C-NMR were used to determine the structure of these molecules. In order to learn more about the structure and vibrational behavior of these compounds, Fourier Transform-Infrared-Attenuated Total Reflectance and Fourier Transform Raman spectroscopy measurements were made in the spectral ranges 600–4000 cm-1 and 0–3500 cm-1, respectively. Additionally, three types of thermal analysis—thermogravimetric analysis (TGA), differential thermal analysis (DTG), and differential scanning calorimetry (DSC)—are used to comprehend the thermal stability of these substances. The poly1-2(Dihydroxyethyl)-3-vinylimidazolium chloride shows important antioxidant properties

Keywords: Vinylimidazolium chloride, DTG, DSC , AIBN

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Non-Orthogonal Multiple Access for Enhanced Cellular Vehicle-to-Everything Communication

Nour El Houda BOUDA[a], SidAhmed ELAHMAR[b]

[a,b] Telecommunications, Telecommunication and Digital Signal Processing Laboratory, Djillali Liabes University, Algeria.

Abstract:

Modern advancements in wireless communication have facilitated real-time information sharing through Vehicle-to-Pedestrian (V2P), Vehicle-to-Vehicle (V2V), and Vehicle-to-Infrastructure (V2I) communications. These technologies encompass a wide range of services, including safety applications for accident prevention, non-safety services for traffic management and efficiency improvement, and infotainment services for user comfort and entertainment. Cellular Vehicle-to-Everything (C-V2X) technology plays a prominent role in this ecosystem by leveraging existing cellular network infrastructure, including base stations, to facilitate communication between vehicles and other entities. This provides wider coverage compared to other V2X solutions. C-V2X utilizes sensors embedded in vehicles to transmit and receive information through the base station, enabling communication with other vehicles, traffic management systems, and even pedestrians. This makes C-V2X particularly suitable for scenarios where long-distance communication between vehicles and infrastructure is crucial. However, integrating Non-Orthogonal Multiple Access (NOMA) holds significant potential to revolutionize C-V2X networks. NOMA allows multiple users to transmit data simultaneously within the same resource block, leading to increased network capacity and enabling denser deployments of vehicles and sensors. Additionally, NOMA's ability to handle superposition coding and successive interference cancellation makes it particularly beneficial for applications demanding high system throughput, low latency, and extended sensor

lifespan. This paper delves into the potential benefits and challenges of utilizing NOMA in C-V2X networks by analyzing the Bit Error Rate (BER) performance under dynamic channel conditions. These dynamic conditions reflect the real-world variations in signal strength and interference that C-V2X systems experience. By analyzing the BER, this work investigates how NOMA affects the reliability and efficiency of C-V2X communication in dynamic scenarios.

Key words: Non-Orthogonal Multiple Access, V2X, C-V2X.

Corresponding Email: boudanoor@gmail.com.
Acknowledgment: This work was supported by the Directorate General for Scientific Research and Technological Development (DGRSDT).

References

[1] CHEN, Shanzhi, HU, Jinling, ZHAO, Li, et al. Cellular vehicle-to-everything (C-V2X). Springer Nature, 2023.

[2] ALALEWI, Ahmad, DAYOUB, Iyad, et CHERKAOUI, Soumaya. On 5G-V2X use cases and enabling technologies: A comprehensive survey. Ieee Access, 2021, vol. 9, p. 107710-107737.

[3] ALLOUIS, Alain, HAMZA, Anis Amazigh, DAYOUB, Iyad, et al. Maximum Sum Rate of MCM-NOMA in Future Vehicular Sensor Networks. IEEE Sensors Letters, 2023.

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Title: Comparative Evaluation of Mechanical Properties of Virgin and Recycled Polypropylene after Aging

[a]Benaichouba Zahira' *Department of Mechanical Engineering, University of* of Mustapha Stambouli , Mascara ,Algeria
[b]Bouziane 'Mohammed Mokhtar *Department of Mechanical Engineering, University of* Dr Moulay Tahar , Saida , Algeria
[c]Bouiadjra Bachir ' *LMPM, Department of Mechanical Engineering, University of Sidi Bel Abbes* [3], Algeria

Abstract:

This study aims to compare the mechanical properties of virgin and recycled polypropylene after exposure to simulated aging conditions. Polypropylene is a widely used polymer in various applications due to its mechanical properties and chemical resistance. However, recycling of polypropylene can affect its properties, raising questions about its long-term durability and reliability. Samples of virgin and recycled polypropylene were subjected to accelerated aging conditions for a period of 3 days and 14 days. Aging conditions included exposure to heat, UV light, and other simulated environmental factors. After this period, tensile and flexural tests were conducted to assess changes in the mechanical properties of the samples .The results of this study will provide crucial insights into the durability and stability of mechanical properties of recycled polypropylene compared to virgin polypropylene after exposure to aging conditions. This information is essential for making informed decisions regarding the use of recycled polypropylene in various

applications, as well as guiding efforts to improve recycling processes and optimize the sustainability of plastic materials.

Key words: .Aging , .polypropylene, ..Virgin, Recycled , Tensil , Flexural .

Corresponding Email: zahira.benaichouba@univ-mascara.dz

Reference

[1] S. Krishna Satya, P.S. Rama Sreekanth, An experimental study on recycled polypropylene and high-density polyethylene and evaluation of their mechanical properties, Materials Today: Proceedings 27 (2020) 920–924

[2] Beatriz L. Fernandes, J. Antonio Domingues, Mechanical characterization of recycled polypropylene for automotive industry, Page 1, Polym. Sci. Technol., 2007, 17 (2): 85–87.

[3] M. Raj, H. Patel, L. Raj, N. Patel, Studies on mechanical properties of recycled polypropylene blended with virgin polypropylene, Int. J. Sci. Invent. Today 2,,2013, (3): 194–203.

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Title: Structural, electronic and magnetic properties of inverse-Heusler alloys Mn_2ZrGe: A first-principles investigation.

Abdelhamid chellali[1], Laboratory of Biomaterials and Transport Phenomena (LBMPT), University Yahia Fares of Medea,Algeria.

Malika amari[2],Laboratory of Renewable Energy and Materials (LREM). University Yahia Fares of Medea, 26.000, Algeria.

Zakaria Triki[1], Laboratory of Biomaterials and Transport Phenomena (LBMPT), University Yahia Fares of Medea,Algeria.

Abstract:

In recent years, Heusler compounds have been investigated due to their useful applications in green energy-related fields, such as solar cells, thermoelectrics, spintronics, superconductors, magnetic actuators. In this paper we present a study of the basic structural, electronic and magnetic properties of both Heusler family; the so-called inverse-Heusler alloys like Mn_2ZrGe .the calculations were performed by using the CASTEP code as a part of Density Functional Theory (DFT).Our result confirm that Mn_2ZrGe adopts a cubic inverse-Heusler structure, in good agreement with theory. We have found that these compounds are emerging as a promising sub-family for spintronic applications .

Key words: Inverse-Heusler , Density functional theory, Mn_2ZrGe, Mstudio , CASTEP,

Corresponding Email:

abdelhamidchellali26@gmail.com

References

[1] Ferhat T, Murat A, Osman C, Selçuk K and Nazmiye K. Half-metallicity in the inverse Heusler Ti2RuSn alloy: A First principles prediction, Journal of Magnetism and Magnetic Materials.

P-107

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Structural &Magnetic Properties of DMS

[1,] Nadjet ZEGGAI,[2] Mostefa DJERMOUNI ,[1] Chaimaa Mohammed krarroubi,

[1] *Département de Physique, Faculté des Sciences et Technologies, Université Ahmed ZABANA de Relizane*
[2]*Département de Physique, Faculté des Sciencesexactes, Université Djilali Liabès de Sidi Bel-Abbès*
Corresponding author: zeggainadjet17@gmail.com

Abstract:
In all the prototype dilute magnetic semiconductor materials (DMS) of groups III-V and II-VI, such as GaAs or ZnO doped with Mn, the maximum Curie Temperature (TC) remains limited to 180-200 K [1] . So far, the magnetic mechanism is not fully understood. These difficulties could be overcome in the recently discovered family of semiconductors (SC) I-II-V [2] and I-III-IV. In these families of SCs, the manipulation of charge and spin is independent. In contrast, the record TC value reported for Ferromagnetic III-V Semiconductors doped with Iron (Ga, Fe) Sb, reaches 340 K, restoring hope in DMS projects. These materials have certain advantages over those doped with Mn. In addition, the similarity between SC III-V GaSb with I-III-IV semiconductors (NaGaSi) gives us the idea to look for an Iron-based DMS which can present an ease of characterization with a Curie temperature relatively high. To achieve this goal, we used DFT theory to describe the electronic structure of the proposed DMS.
Key words: DMS , DFT , Magnetic

Corresponding Email:

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Marine Algae-Derived Activated Carbon: A Sustainable Solution for Pollutant Removal.

Abir BENHADDA, Sarra BOURAHLA[b],Fadela NEMCHI[c].

[a] Department of marine science, university of mostaganem, Mostaganem, Algeria.
[b] Department of chimestry, university of mostaganem, Mostaganem, Algeria.
[c] Department of marine science, university of mostaganem, Mostaganem, Algeria.

Abstract:

Marine algae, often overlooked as an underexploited bioresource for centuries, are primarily recognized for their natural polysaccharides. Their utilization has expanded across numerous fields, including the pharmaceutical, cosmetic, and food industries, and more recently in water treatment as biosorbents. This study delves into the efficacy of marine macroalgae for contaminant removal from water. An activated carbon is prepared from the brown alga ***Cystoseira stricta*** using chemical activation and thermal treatment. Dried algae were impregnated with phosphoric acid and subsequently activated at 800°C for one hour. The resulting carbon powder was characterized by FT-IR spectroscopy and analyses of methylene blue and iodine indices. The findings demonstrate that activated carbon produced from dried brown algae holds promise as an economical and effective alternative for pollutant removal in water.

Key words: Marine algae, bioresources, activated carbon,water contaminants.

Corresponding Email: abir.benhadda.etu@univ-mosta.dz.

P-109

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Title: Structural, electronic and thermoelectric properties of antiperovskite compound Sr_3SiO: A first principles study

BLAHA Lamia Farah[a], KHATIR Radja[b], AMERI Ibrahim[c],

[a]Laboratory of Physical Chemistry of Advanced Materials (LPCMA), University of Djillali Liabes, Sidi-Bel-Abbes, Algeria.
[b]Laboratory of Electrical Engineering and Materials (LGEM), The Higher School of Electrical and Energetic Engineering (ESGEE), Oran, Algeria.
[c]Laboratory of Physical Chemistry of Advanced Materials (LPCMA), University of Djillali Liabes, Sidi-Bel-Abbes, Algeria

Abstract:

In the last years, alkaline-earth based antiperovskite compounds with small semiconductor band gap have been proven to be promising candidate for optoelectronic and thermoelectric applications. In this work, the structural, electronic and thermoelectric properties of Sr3SiO compound have been predicted using first principles calculations based on the full-potential linearized augmented plane-wave (FP-LAPW) method and semiclassical Boltzmann transport theory. Exchange-correlation effect is treated with the generalized gradient approximationwith Perdew–Burke–Ernzerhof scheme (GGA-PBE) and Tran–Blaha modified Becke–Johnson exchange potential. Sr3SiO is a semiconductor with direct band gap of 0.328 eV. Finally, the thermoelectric properties including Seebeck coefficient, electrical conductivity, thermal conductivity, power factor and figure of merit are calculated. Obtained results show that Sr_3SiO could be candidate for applications in thermoelectric generators at low and moderate temperatures due to their high figure of merit values.

Key words: ab initio, GGA –mBJ , semiconducting, antiperovskites, thermoelectric properties,

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Title: Ab-initio predictions of Structural, electronic and magnetic properties of double-Ge-layer MAX phase Cr2Ge2C.

Henen BERROUNA[a,*], Yahia AZZAZ[b], Yamani MASSIM[c]

[a] Department of Physics, Faculty of Exact Sciences, Laboratory of Physico-Chemistry of Advanced Materials, University of Sidi Bel Abbes, 22000, Algeria
[b] Laboratory of Physico-Chemistry of Advanced Materials, University of Sidi Bel Abbes, 22000, Algeria
[c] Laboratory of materials for application and valorization of renewable energies (LMAVER). University of Laghouat, Algeria

Abstract:

The magnetic stability and electronic properties of a new MAX phase Cr2Ge2C are investigated using density functional theory (DFT) with the generalized gradient approximation GGA and GGA+U. our work conducted predictive calculation of new nanolaminate Cr2Ge2C followed comparison with Ge-containing M2AX phases, the magnetic ground states are predicted as NM with GGA approximation and AFM configuration with GGA+U method. Our result has shown that the total and partial magnetic moment are greatly decreased rapidly to zero by adding Ge layer. Due to the extra Ge-layers, the TDOS of the Cr2Ge2C at the Fermi level reduces slightly compared with Cr2GeC and the Cr–C bond becomes more covalent compared with another study in Cr2GeC. Finally, we hope that the theoretical study of the new MAX phase material is the first of a large family, which will give a plus in the future for experimenters and theoreticians.

Key words: DFT, New MAX Phase, M2A2X compound. GGA+U.

References

[1] Hu C, Lai C-C, Tao Q, Lu J, Halim J, Sun L, Zhang J, Yang J, Anasori B, Wang J, Sakka Y, Hultman L, Eklund P, Rosen J, Barsoum MW (2015) . Chem Commun 51(30):6560–6563
[2] Lai CC, Meshkian R, Dahlqvist M, Lu J, Na¨slund LA˚ , Rivin O, Caspi EN, Ozeri O, Hultman L, Eklund P, Barsoum MW, Rosen J (2015). Acta Mater 99:157–164
[3] Horlait D, Grasso S, Chroneos A, Lee WE (2016). Mater Res Lett. Vol. 4, No. 3, 137–144,

* Corresponding Email: berhenen@yahoo.fr

P-111

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Synthesis and Characterization of $CeNiO_3$ Perovskites to Nitrophenol Degradation

Fouzia Abderrahmani,[a] Nadia Aider[a], FouziaTouahra[c], BayaDjebarri[b], Nouara Lamrani[a]

[a] *Laboratoire de Chimie Appliquée et de Génie Chimique (LCAGC), Université Mouloud Mammeri, 150 0 0, Tizi-Ouzou, Algeria*

[b]*Laboratory of Applied Chemistry and Materials (LabCAM), University of M'hamed Bougara of Boumerdes, Avenue de l'Indépendance Boumerdes, 35000. Algeria*

[c]*Centre de Recherche Scientifique et Technique en Analyses Physico-chimiques (CRAPC), BP 384-Bou-Ismail,RP42004, Tipaza, Algeria*

Abstract:

Treating contaminated waste wáter is a crucial environmental protection measure. Industries such as paint, pharmaceutical, and chemical emit organic matter and discharge effluents loaded with soluble and insoluble pollutants daily. However, it is often neglected. Industries such as paint, pharmaceutical, and chemicalemitorganicmatter and discharge effluents loadedwith soluble and insoluble pollutants daily. Nitro-aromaticcompounds are classified as toxic substances for reproduction and are amongthe pollutants. The text discusses the reduction of Nitrophenol (NP) to Aminophenol (AP) duetothetoxicity of NP and the industrial and pharmaceuticalapplications of AP.

Mixed oxides in photocatalysis in aqueous media have shown promise. The irorganised structure,large specific surface area, termal stability, and interesting physical and chemical properties make them ideal.

We synthesise dhigh-performance catalysts, such as $CeNiO_3$-type perovskites, using two preparation methods: co-precipitation and sol-gel. The two materials were characterised by XRD. The wave length of 365nm is used for the reduction of nitrophenol by photocatalysis.

The text describes the influence of pH, nitrophenol concentration, and catalyst mass on nitrophenol reduction.

Key Words: *Nitophenol, perovskites, sol-gel, co-precipitation, photocatalysis.*

Corresponding autor Email: fouzia.abderrahmani@fs.ummto.dz

References

[1]I. Jung, H.-Y Jeong, J.-S. Lee, M. G. Kim, J. Cho, Angew. Chem. 2014, 126, 4670 –4674

[2] J. Suntivich, K. J. May, H. A. Gasteiger, J. B. Goodenough, Y. Shao-Horn, Science, 2011, 334, 1383-1385

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Green synthesis of ZnO nanoparticles from castor oil leaf extract: Environmental use, kinetic and thermodynamic studies of adsorption of a toxic dye.

Mohammed Cherif TERKHI[a], Kinza Amel BELHADJI[a], Sabria TERKHI[b], Mouffok Radouane GHEZZAR[a], Fatiha ABDELMALEK[a], Ahmed ADDOU[a]

[a]Laboratory of Environmental Sciences and Techniques (STEVA), Faculty S.T, Univ. of Mostaganem, Algeria.

[a]Laboratory of Solid Technology and Property, Faculty S.T, Univ. of Mostaganem, Algeria.

Abstract:

The presence of micropollutants in water resources, such as dyes, makes it necessary to develop new water and wastewater treatment methods. This is why research into green nanoparticles is underway, due to their lower cost and effective adsorption properties. This work therefore describes the environmentally friendly production of Zinc oxide nanoparticles (ZnO-NP) derived from a Ricin leaf extract, used to remove a toxic organic dye Gentian Violet (GV). The physico-chemical properties of ZnO-NP were determined using BET, FTIR and SEM analyses. The effect of experimental parameters such as contact time, ZnO-NP dose, pH, initial concentration and temperature was studied. The large specific surface area of the ZnO-NP adsorbent, the presence of pores and the negative surface charge make it an interesting tool for removing this cationic dye GV. The pseudo-second-order model was fitted by the kinetic data, which took 40 minutes to reach equilibrium. A maximum adsorption capacity of 190 mg/g was found by the equilibrium search, and the experimental data best fit the Langmuir model. Thermodynamic parameters showed that GV adsorption was an exothermic and spontaneous process. Based on these results, ZnO-NP offers great potential for application in the treatment of dye-contaminated water.

Key words: Nanoparticules ZnO; Castor oil leaves; Gentian Violet; Green Chemistry

Corresponding Email : mcterkhi.univmosta@gmail.com

References

[1] Singh, Nahar, et al. "Green synthesis of zinc oxide nanoparticles using lychee peel and its application in anti-bacterial properties and CR dye removal from wastewater." Chemosphere 327 (2023): 138497.

[2] Asjadi, Fatemeh, and Maliheh Yaghoobi. "Characterization and dye removal capacity of green hydrothermal synthesized ZnO nanoparticles." Ceramics International 48.18 (2022): 27027-27038.

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Analysis of the effect of aging duration in water immersion of a damaged structure repaired by the bonding process.

M. Benyettou [a*], K. Madani [a], S. CH. Djebbar [a] , M. Belhouari [a], A.Houari[b].

[a]Mechanical Engineering Department, Djillali Liabes University, Algeria
[b]Mechanical Engineering Department, University of Boumerdes, Algeria

Abstract:

Since the implementation of the composite or metallic patch repair process in various industrial sectors to increase the strength of damaged structures, this method has rapidly expanded for use in other fields such as civil and naval engineering, etc…. Despite the numerous advantages of this technique, it is only applicable to secondary structures because during the service life, the repaired structure is simultaneously exposed to mechanical and environmental stresses, causing a considerable decrease in the mechanical properties of the adhesive and the composite [1-2]. Current research aims to characterize these two materials under severe conditions to estimate their usage and prevent rapid failure of repaired structures. Our work falls within this context. The objective is to analyze, using the finite element method, the fracture behavior of a damaged 2024-T3 Aluminum structure repaired by a patch under aging effects. The effect of crack length, single and double patch repair, patch material, and aging duration has been highlighted on the global behavior of the structure. The results clearly show that the mechanical properties degradation of the repair patch and the adhesive significantly affect the value of the J-integral and consequently the strength of the repaired structure.

Key words: . Aluminum 2024-T3, adhesive, single and double patches, ageing, J-integral.

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Comprehensive Analysis of the Structural, Electronic, Elastic Properties of ternary chalcogenides pnictogens $InPnS_3$ (Pn=Bi, Sb) Compounds: First-Principles Calculations.

A. Benarroudj[a,b], M. Bouchenafa[a,b], S. Maabed[a,b], O. Arbouche[c].

[a] Laboratory of materials for applications and valorization of renewable energies (LMAVER), University Amar Telidji Laghouat, Algeria
[b] Department of Material Sciences, Faculty of Sciences, Amar Telidji University, BP 37G, Laghouat, 03000, Algeria
[c] Laboratory Physico-Chemistry of Advanced Materials, Djillali Liabes University of Sidi Bel-Abbes, 22000 Sidi Bel Abbes, Algeria

Abstract:

Semiconductors with a wide gap energy band are essential for today's electronic devices [1] [2] as well as for various applications of energy conversion [3] [4] and water splitting [5]. The chalcogenides $InPnS_3$ (Pn = In, Bi) are promising candidates, because they are materials made of elements abundant on earth and non-toxic. In this work, we present a study based on density functional theory to access structural, electronic and elastic properties. Band structure and DOS analysis show that all of these materials are indirect gap semiconductors, with a gap band energy (HSE06) of 2.065 eV and 2.45 eV for $InSbS_3$ [6] and $InBiS_3$ [7], respectively. The elastic properties of these materials strongly depend on the direction thus manifesting an anisotropic character, where the direction of the y axis presents the highest values ($C_{22} > C_{11}$ and C_{33}). In addition, with a Pugh ratio B/G < 1.75 [8] our materials are considered fragile. According to our calculations, the $InBiS_3$ material has the best elastic properties with a bulk modulus of 37.22 GPa, a Young modulus of 53.35 GPa and a shear modulus of 21.15 GPa.

Key words: Chalcogenide, DFT, semiconductor, optoelectronic, sulfide.

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

A Robust Interval Type-2 Fuzzy Logic Controller of a Doubly Fed Induction Generator for Wind Energy Conversion

[1]Izzedine Allali[a], Boubekeur Dehiba[b]

a Laboratoire IRECOM Université Djillali Liabes, de Sidi Bel-Abbes,Algérie
[b] Laboratoire IRECOM Université Djillali Liabes, de Sidi Bel-Abbes,Algérie

Abstract:

This study details a method for controlling a wind energy conversion system that uses a doubly-fed induction generator and interval type-2 fuzzy logic. Using a nonlinear control rule provides the clearest rationale for this strategy when dealing with model uncertainty concerns. The purpose of this command is to regulate the flow of reactive and active power from the doubly-fed induction generator to the network, which will then act on the signals from the rotors through a bidirectional converter. Various operating situations, including variable speed generation and parameter modification, are used to evaluate the effectiveness of the suggested control technique.

Using metrics like track references, settling time, and overshoot value, the simulation findings show that the interval type 2 fuzzy logic controller is more resilient than the T1 FLC. The simulations were performed using MATLAB/Simulink software

Keywords – Doubly fed induction generator, wind power, IT2-FLC, T1-FLC

1. Introduction

As a sustainable and eco-friendly energy source, wind power has grown substantially during the last decade [1-2]. Renewable energy has seen a dramatic uptick in research and development within the last decade. This is because, as fuel supplies have become increasingly scarce, the cost of producing power using more conventional means has risen. Furthermore, environmental concerns related to thermal and nuclear power generation have grown in public consciousness. Wind power generating systems (WPGS) are among the most cutting-edge and long-standing green power solutions for harnessing wind energy. Worldwide, wind power has the potential to provide more energy than one gigawatt (GW), and even more massive wind farms are under construction [3-4-5].

Currently, the majority of wind turbines have a DFIG installed because of its many benefits: variable speed production (with a ± 30% variation around the synchronous speed), separated control over active and reactive power, less noise and mechanical stress, enhanced power quality, and cheap cost [6].

azziz.allali46@gmail.com

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Activation of persulfate by several methods to degrade polyphenols contained in olive mill waste water

Rabea SEMANE[a], Hamida IBOUKHOULEF[b] , Abdelhamid ELIAS[c]

Laboratoire de Chimie Appliquée et de Génie Chimique, Université Mouloud Mammeri- Tizi-Ouzou,Algérie
Laboratoire de Chimie Appliquée et de Génie Chimique, Université Mouloud Mammeri- Tizi-Ouzou, Algérie
Laboratoire de Chimie Appliquée et de Génie Chimique, Université Mouloud Mammeri- Tizi-Ouzou, Algérie

Abstract: Olive oil production is an important part of economic activity in Mediterranean area.
Even though the olive oil industry is one of the most important sectors benefiting economically the producing countries, it generates one of the most polluting wastewaters: the olive mill wastewater (OMW) .
OMW poses severe problems for environmental systems, especially in the Mediterranean region;
therefore, its treatment is of great interest. A wide range of treatment technologies have been evaluated by researchers for the treatment of OMW, among them, advance d oxidation process (AOPs) is receiving great attention [1]. AOPs are mainly based on the production of nonselective and highly reactive free radicals. Nowadays, sulfate radical treatment using persulfate (PS) or peroxy monosulfate (PMS) have gained prominence in the removal of organic contaminants, as well as in water and wastewater treatment. Persulfate is advantageous in many ways such as being solid at room temperature , being easily stored and transported and having high stability, water-solubility and low cost. Persulfate is a strong oxidizing agent with a redox potential of 2.20 and long half time compared to hydroxyl radical. Vary activation methods were used to generate sulfate radicals from precursors including heat, transition metal ions, ultra-violet (UV) light, etc.,
it can form highly reactive sulfate radicals that have a higher redox potential (2.60V) [2].
In this work, persulfate (PS,$S_2O_8^{2-}$) was activated by several methods to produce sulfate radical (SO_4^{-}). The combined effect of independent parameters (persulfate and copper concentration, treatment time, temperature, initial pH and activation mode) on phenolic compounds removal efficiency was investigated and optimized using a screening with Hadamard matrix.
The results obtained made it possible to obtain a reduction of phenolic compounds of 59% with
the combination of ozone and thermal activation for PS.

Key words: olive mill wastewater, abatement, persulfate oxidation, ozonation, Hadamard matrix.

Corresponding Email: rabea.semane@fs.ummto.dz

References

[1] H. Iboukhoulef, A. Amrane, H. Kadi, Removal of phenolic compounds from olive mill wastewater by a Fenton-like system H2O2/Cu(II)—thermodynamic and kinetic modeling, Desalination and Water Treatment, 57 (2014) 1874-1879.

[2] M. Forouzesh, A. Ebadi, F. Abedini, Thermocatalytic persulfate activation for metronidazole removal in the continuous operation, Separation and Purification Technology, 258 (2021) 118055

P-117

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Effect of ultrasound, microwave assisted extraction on seaweeds material

Kahina Hamamouche[a], Zoubida Elhadj[b], kalouche Moustafa[a] Latifa khatabi[c], Nossaiba chafaa[e], Rachid Meghabar[b]

[a], Environmental Monitoring Network Laboratory, Département of biologie, Université of Ahmed Ben Bella Oran-1, Algérie.
[b] Laboratoire of sience stady of Environment and Material, Département of Chemistry, Université of Ahmed Ben Bella Oran-1, Algérie.
[c]Biotechnology Research Center, Ali Mendjli Nouvelle Ville UV 03 BP E73, Constantine 25016, Algeria.
[e]Laboratory of natural substances, biomolecules and biotechnological applications, Département of sciences of nature and life, university of Larbi Ben M'hidi, Oum El Bouaghi, 04000, Algeria.

Abstract:

Notable technological advances are visible, but the task ahead is to preserve growth by adopting environmentally friendly technologies. One of tools to achieve this goal is to use non-traditional technologies, commonly referred as advanced technologies. The objective of this study is to compare the effectiveness of two techniques, microwave-assisted extraction (MAE) and ultrasonic-assisted extraction (UAE), for extracting bioactive compounds from red and brown algae, respectively Jania rubens and Sargassum muticum sample on the west coast of Algeria. Our research shows that total phenolics are higher by the UAE method. The values recorded for the tests: 2,2-diphenyl-1-picrylhydrazyl (DPPH) and ABTS showed exceptionally high antioxidant activity with UAE.Nevertheless, Phenanthroline test gives superior results by MAE. In conclusion, the choice of extraction method is determined by different criteria, including the type of species, sampling duration, solvent and time extraction. Due to their low environmental footprint, so considered as eco-friendly.

Key words:*Jania ruben, Sargassum muticum,* biological activity, microwave Assisted Extraction, ultrasound Assisted Extraction .

Email: hamamouche.kahina@edu.univ-oran1.dz

References

[1] Ummat, V., et al., Advances in pre-treatment techniques and green extraction technologies for bioactives from seaweeds. Trends in Food Science & Technology, 2021. 110: p. 90-106.

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Electrochemical studies of anodic oxide films on titanium and TA6V alloy

Hayette BOUTARFA [1,2], Salih HAMDI [1,2], Samah ADJMI [1,2] .

[1]Department of Physics, Faculty of Science and Technology, Unversité Chadli Bendjedid, 36000 El Tarf, Algeria.
[2]Physico-chemical laboratory of materials, sciences and technologies, Chadli Bendjedid University, 36000 El Tarf, Algeria.

Corresponding author's: boutarfa-hayette@univ-eltarf.dz

Abstract

Titanium and its alloys have attractive characteristics (good corrosion resistance, high mechanical characteristics, low density, transformation by conventional processes, etc…). They are used in the chemical engineering, the automobile, the marine applications aerospace, military, and biomedical industries, especially Ti-6Al-4V alloy. In this work, we carried out an experimental study of the electrochemical mechanism of cerium oxide on a Ti-6Al-4V substrate. (Titanium 90%, Aluminum 6% and Vanadium 4%, Titanium grade 5), was prepared by electrodeposition from dissolution of cerium nitrate Ce(NO3)36H2O in a mixed ethanol solution (50% water and 50% ethanol) at a concentration of 0.01 mol.l-1. The deposits were produced at room temperature at 21 degrees , during different electrodeposition times (900s, 1800s and 3600s) by imposing different current densities: -0.5, -1 and -2 mA/cm². We used X ray diffraction analysis (XRD) to characterize the engineered coatings.

Keywords: Electrochemical studies, anodic oxide films, Ti-6Al-4V and X-ray diffraction analysis (XRD).

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Modeling of Drug-Protein Binding Fraction (FB) by CNN-MLP

Abdellah Ibrir [a,b], Mohamed Hentabli [b], Zineb Haddouda [b], Safaa Boukerma [b], Hakim Bouzemlal [b], Latifa Khaouane [b].

[a] Department of Process Engineering, University Saad Dahlab Blida1, Physical Chemistry of Material Interfaces Applied to the Environment (PCMIAE), Blida, Algeria
[b] Department of Process Engineering, University Yahia Fares of Medea, Laboratory of Biomaterials and Transport Phenomena (LBMPT), Médéa, Algeria

Abstract:

This study was conducted to compare different methods for predicting the drug-protein binding fraction (FB), a key pharmacokinetic parameter. For this, molecular descriptors from RDKIT for 263 active substances were calculated. Machine learning techniques, including Artificial Neural Networks (ANN) and Support Vector Machines enhanced by the Dragonfly Algorithm (DA-SVM), were employed. The models were trained using a dataset refined through a genetic algorithm (GA), with the reduced dataset used for both ANN and DA-SVM models. Innovative deep learning approaches were also explored, such as Convolutional Neural Networks with Multi-Layer Perceptron (CNN-MLP) and Convolutional Neural Networks with DASVM (CNN-DASVM). Notably, strong predictive performance and robustness were achieved with the CNN-MLP model, which yielded R^2 values of 0.99 and RMSE = 0.042. These results show the robustness of the mathematical model established.

Key words: drug-protein binding fraction, descriptors, Machine learning techniques, genetic algorithm, deep learning, Convolutional Neural Networks.

Corresponding Email:
ibrir.abdellah@yahoo.com

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Ab initio electronic structure and magnetism in Sr2MOsO6 (M= Cu or Ni) double perovskite systems: a GGA+U and GGA + U +SOC

Kheirallah mohammed[1,2], Bensaid Djilali[b]

[1] Department of Subject Sciences, Faculty of Science and Technology, Belhadj Bouchaib Aintemouchent University
[2] magnetic materials laboratory UDL Sidi Bel Abbes
[b] Automatic Department, Faculty of Electrical Engineering,UDL SBA

Abstract:

The electronic and magnetic properties of the tetragonal double perovskite Sr2MOsO6 (M = Cu, Ni) were investigated using density functional theory (DFT) calculations, which incorporated spin-orbit coupling (SOC). This approach allowed for a comprehensive analysis of the electronic structure and magnetic behavior of Sr2MOsO6 (M = Cu, Ni), taking into account the effects of relativistic interactions between electron spins and their orbital motion (spin-orbit coupling). The ordered double-perovskites Sr2MOsO6 (M = Cu, Ni) consisting of 3d and 5d transition-metal magnetic ions (M (2+) and Os (6+), respectively) are magnetic insulators.

Key words: double lead-free perovskite, optoelectronics, DFT and ferromagnetic

Corresponding Email: mohammed.kheirallah@univ-temouchent.edu.dz

---

References

[1] Near compensated half-metal in Sr2NiOsO6 Weiyu Song,[1,2] Erjun Zhao,[1,2] Jian Meng,[1] and Zhijian Wu[1,a]

[2] Half metallic properties of Sr2CuOsO6 Weiyu Song [a, b], Jing Wang [a,b], Zhijian Wu [a,*]

P-121

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Title: Half-metallic ferrimagnetic characteristics of Ti_2-based ternaryHeusler alloys.

M. Drief[1,2] Y. Guermit[1,3] K.Houcin[3], H.Rekab djabri[2], T.Antri[3], H. Rached[1,4] D. Rached[1,5] , N.Benkhatou[1,5]

Abstract:

Heusler alloys are predicted from a theoretical point of view to evolve into half-metals at room temperature (RT). Their three main assets are their suitable lattice matching irrespectively to the substrates, their high Curie temperature over RT, and the possibility to tune their intermetallic character for spin density of states at the Fermi energy level. The investigation of the magneto-electronic properties along with the structural, mechanical, and thermoelectric characteristics of a novel Ti_2-based ternary Heusler alloy Ti_2RuZ (Z = Si, Ge, Sn) family through the full-potential linearized augmented-plane-wave method (FP-LAPW) based on the Wien2k program is reported. The structural, magnetic, and electronic properties revealed that these compounds are ferrimagnet (FiM) materials. Due to the predicted and calculated negative formation energy, these investigated compounds could be thus synthesized experimentally. The mechanical study shows that these Ti_2-based ternaryHeusler alloys are stable against any elastic deformation and belong to the brittle and stiff material category. The half-metallic ferrimagnet (HM-FiM) behavior was confirmed from the magneto-electronic calculations for all the investigated compounds. Furthermore, the thermoelectric responses as a function of chemical potentials and temperatures were analyzed and revealedthat the new investigated alloys display a high figure of merit, a large Seebeck coefficient conjugated to low thermal conduc-tivity. The present study proposes these compounds as potential candidates for spintronic thermoelectric devices.

Key words: Ab initio calculations · Heusler alloys · HM-FiM compounds · Thermoelectric response

1 **Magnetic Materials Laboratory (LMM), Faculty of ExactSciences, Djillali Liabes University of Sidi-Bel-Abbes, Sidi-Bel-Abbès, Algeria**

2 **SNVT, university bouira,Algerie**

3 **ST University relizane.Algeria**

4 **SE University chlef,Algeria**

5 **SE University sidi bel abess ,Algeria**

Corresponding Email:m.drief@univ-bouira.dz

P-122

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Effects of nitrogen incorporation on the optoelectronic properties of BSb binary compound: Optoelectronic application

Djamel BOURAGBA[*a], Miloud BENCHEHIMA[a,b], Kada BENCHIKH[a] and Hamza ABID[a]

[a]*Applied Materials Laboratory, Research Center (CFTE), Sidi Bel Abbès Djillali Liabes University, 22000, Algeria*
[b]*Electronic Department University of Sciences and Technology of Oran, Mohamed Boudiaf (USTO), El M'nouar BP 1505, Oran, Algeria*

Abstract:

Optoelectronic properties of $BSb_{1-x}N_x$ ternary alloys in zinc blende structure are investigated by employing the first-principles calculations based on the density functional theory. We have evaluated $BSb_{1-x}N_x$ ternary alloys using special quasi-random structures with 8 atoms. The generalized gradient approximation of Perdew et al. (PBEsol-GGA) was used as the exchange correlation potential to calculate the structural properties at different nitrogen concentrations x ($0 \leq x \leq 1$). The structural parameters *have* been evaluated and analyzed. Our obtained results show that the lattice parameter of $BSb_{1-x}N_x$ decreases with nitrogen concentration (x) while its bulk modulus increases. The electronic properties were predicted using the Tran–Blaha-modified Becke–Johnson (TB-mBJ) scheme. The band gap of $BSb_{1-x}N_x$ positively deviates from Vegard's law. The optical response functions are determined for $BSb_{1-x}N_x$. In general, our results are in agreement with the available experimental and theoretical data reported in the literature. The calculation endorses that the $BSb_{1-x}N_x$ ternary is a promising candidate for optoelectronics.

Key words: BSb binary compound; Zinc blende structure;Density functional theory; Optical properties;

Corresponding Email: bouragba.djamel@yahoo.fr

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Mesoporous silica doped with AgNPs/CeO_2 nanoparticles for water pollutant reduction.

Fatima HABECHE[a,b], Bouhadjar BOUKOUSSA [b,c], Fadila BENALI [b], Adel MOKHTAR[b,d], Mohammed HACHEMAOUI[b,e]

[a] Science and Technology Field, Institute of Science and Technology, Ahmed Zabana University, 48000 Relizane, Algeria
[b] MaterialsChemistry Laboratories L.C.M, University Oran1 Ahmed Ben Bella, BP 1524, El-Mnaouer, 31000 Oran, Algeria
[c] Department of Materials Engineering, Faculty of Chemistry, University of Sciences and Technology Mohamed Boudiaf, BP 1505, El-Mnaouer, 31000 Oran, Algeria
[d] Process Engineering Departments, Institute of Science and Technology, Ahmed Zabana University, 48000 Relizane, Algeria
[e] Department of Material Sciences, Institute of Sciences and Technologies, Ahmed Zabana University, 48000 Relizane, Algeria.

Abstract:

The charged wastewater is often discharged into the natural environment without effective treatment, which can have adverse effects on the ecosystem and human health. Dyes are among the pollutants contained in industrial waste and wastewater. In this work, the mesoporous silica MCM-41 was prepared by a hydrothermal method and then modified using silver and copper. The obtained samples were used as catalysts for the reduction of the following dyes: Methylene Blue (MB), Congo Red (CR), Methyl Orange (MO), and Orange G (OG). Several parameters affecting the reduction of dyes were investigated and discussed such as the catalyst nature, the initial concentration of the dye, the dye nature, the selectivity of the catalyst in a binary system as well as the catalyst reuse. The analysis clearly showed that the calcination of copper- and silver-modified silica leads to the formation of well-dispersed CuO and AgNPs having sizes between 5-10 nm. As determined by XRF analysis, the content of silver nanoparticles was higher compared to CuO in all samples. It has been

shown that the dye reduction is influenced by the size and the content of nanoparticles as well as by their dispersions. The catalytic activity was shown to be the highest for the Ag-Cu-MCM(0.05) catalyst with a rate constant of 0.114 s^{-1}, 0.102 s^{-1}, 0.093 s^{-1}, and 0.056 s^{-1}, for MO, MB, CR and OG dyes in the single-dye system, respectively. In the binary system containing MB/OG or MB/MO, the catalyst Ag-Cu-MCM (0.05) was more selective towards the MB dye. The reuse of the catalyst for three consecutive cycles showed higher MB conversion in a single system with an increase in reaction time.

Key words: wastewater,dyes, MCM-41, Ag-Cu-MCM-41,catalytic reduction

Corresponding Email:

habeceheamel@yahoo.fr

References

[1] Behera M, Nayak J, Banerjee S et al (2021) A review on the treatment of textile industry waste effluents towards the development of efficient mitigation strategy: an integrated system design approach. *J Environ Chem Eng* 9:105277

[2] Shenoy A, Shukla BK, Bansal V (2022) Sustainable design of textile industry effluent treatment plant with constructed wetland. *Materials Today: Proceedings*

P-124

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

New method of valorization of natural materials and their applications.

Zahraoui Mehdi[a], Derkaoui Fatma[b], Sassi Mohammed[c]

[a]Zahraoui Mehdi' Department of Process Engineering,Science and Technology,University of Relizane, Algeria
[b] Derkaoui Fatma' Department of Chimistry, Science and Technology University of Oran1, Algeria
[c] Sassi Mohammed' Department of Chimistry, Science and Technology University of Oran1, Algeria

Abstract:

Tthe Zeolite Y is synthesized by the hydrothermal method using two different sources a commercial source and a natural source , The use of thermally treated metakoiln by sodium carbonate allowed us to obtain well crystallized Zeolite Y. the resulting Zeolite is subjected to the ionic exchange of this Zeolite with nickel nitrate (II) and cobalt nitrate (II) The materials obtained were characterized and applied as antifungal agents This result was confirmed by XRD diffraction, and FTIR spectroscopy Tested as antifungal materials, the Zeolite Y exchanged materials exhibited a good antifungal activity against

Key words: Zeolite Y, Nickel nitrate (II), Ccobalt nitrate (II), Antifungal activity

Corresponding Email:

ezahraoui48@hotmail.fr

References

[1] B. Dizman, J. C. Badger, M. O. Elasri, and L. J. Mathias, Antibacterial fluoromicas: A novel delivery medium. Applied Clay Science. (2007)

[2] M.M. H. Htun, M.M. Htay and M. Z. Lwin, Preparation of Zeolite (NaX, Faujasite) from Pure Silica and Alumina Sources, International Conference on Chemical Processes and Environmental issues (ICCEEI'2012) July, 2012 .

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

PREDICTION OF CORROSION POTENTIAL USING THE GENERALIZED ARTIFICIAL NEURAL NETWORKS METHOD

CHERIFI Wafa Nor El Houda[a*] ; HOUMADI Youcef[b] ; Aissa Mamoune Sidi Mohammed[a]

[a]Smart structures Laboratory (SSL), University of Ain Témouchent, Department of Civil Engineering, PBox 284, 46000 Algeria
[b]Smart structures Laboratory (SSL), University of Tlemcen, Department of Civil Engineering, 22, Rue Abi Ayed Abdelkrim Fg Pasteur B.P 119 13000, Tlemcen, Algérie

Abstract:

Corrosion of reinforcement bars is one of the key phenomena determining the lifespan of a structure. It can be monitored through methods based on various corrosion probability indicators. Some of these measures are more time-consuming and require highly specific equipment. In recent years, several non-destructive tests have been developed to be relatively quick and less costly, based on measuring corrosion potential. In this study, a statistical analysis is conducted using multiple linear regression to test the reliability of data obtained through experimental measurement of corrosion potential using the Canin+ device at Ain Témouchent University. Artificial neural networks (ANN) are then employed to develop a model for predicting the corrosion potential of reinforcement bars in concrete or mortar. Consequently, to develop a model accurately predicting the corrosion state based on corrosion potential, an ANN-based model is presented in this work. A total of six hundred and forty experimentally obtained data points were used for ANN modeling, with 512 data points used for training, 64 for validation, and 64 for testing.

Key words: Corrosion, durability, neural networks, potential.

Corresponding Email: wafa.cherifi@univ-temouchent.edu.dz

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

FIRST PRINCIPLES CALCULATIONS TO INVESTIGATE STRUCTURAL, ELECTRONIC AND THERMOELECTRIC PROPERTIES OF LiZnP HALF-HEUSLER

Sehoul Baghdad[a], Bouguerba Salah Eddine[b], Sehoul Mohammed[c]

[a] Laboratory of Electronic Systems, Telecommunications and Renewable Energy , Nour Bachir El-Bayadh University Center, BP 900 route Aflou, 32000 El Bayadh, Algeria
[b] Department of Science and Technology, Nour Bachir El-Bayadh University Center, BP 900 route Aflou, 32000 El Bayadh, Algeria
[c]Department of Science and Technology, Nour Bachir El-Bayadh University Center, BP 900 route Aflou, 32000 El Bayadh, Algeria

Abstract

Preserving the environment and natural resources, converting heat into electricity and vice versa, building devices sensitive to magnetic fields such as magnetic resistors, building memory cells and many technological applications have increased researcher's interest in research of materials meeting these needs. Among these materials that have achieved great fame in the field of scientific research, we cite heusler compounds and half heusler compounds due to its properties that make it suitable for thermoelectric applications.in this article, and we have highlighted one of these LiZnP compounds. This done by studying its properties, which include structural, electronic and thermoelectric properties. By applying density functional theory using a wien2k [1]. Through the study, we concluded the LiZnP compound is stable in the nonmagnetic phase. It was revealed that this compound is a semiconductor, the energy of gap was calculated based on the generalized gradient (GGA) and the Becke-Johnson approach modified by Tran-Blaha (TB-MBJ) [2]. Which equal 1.38 eV and 1.99 eV respectively according to the two approximations mentioned previously. Additionally, this compound was noted to exhibit high efficacy Figure of merit. ZT has greater effects when the chemical potential is positive.at room temperature the maximum

value of ZT≈1 at 300K. This study demonstrates that the thermoelectric performances at room temperature.

Key words: Half Heusler, Density functional theory, ab-initio calculations, LiZn

Corresponding Email:

Sehoulbaghdad2019@gmail.com

References

[1] BLAHA, Peter, SCHWARZ, Karlheinz, MADSEN, Georg KH, et al. wien2k. An augmented plane wave+ local orbitals program for calculating crystal properties, 2001, vol. 60.

[2] TRAN, Fabien et BLAHA, Peter. Accurate band gaps of semiconductors and insulators with a semilocal exchange-correlation potential. Physical review letters, 2009, vol. 102, no 22, p. 226401.

P-127

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Influence of various heat treatments on elastic parameters of CuZnAl shape memory alloy

Debboub Salima [a,b], Boukhatem Radia [b] and Chouf Saida [a]

[a] Laboratory of Materials Elaboration and Analysis, Badji Mokhtar-Annaba University, Annaba, Algeria
[b] Department of Physics, Chadli Bendjedid University, El Tarf, Algeria

Abstract:

This work is dedicated to the characterization of CuZnAl shape memory alloy using an acoustic technique by means of ultrasonic echography. The experimental device operates in a frequency range from 20MHz to 50MHz to compute the propagation velocities of longitudinal acoustic waves.
The main goal is to show the influence of various heat treatments that are undergone by the alloy on the elastic parameters such as Young's modulus E and the shear modulus G which are linked up to the longitudinal and transverse velocities of the ultrasonic waves with theoretical relations.
In fact, heat treatments changes both the crystalline structure of the alloy at high and low temperature. Some processing lead to martensitic change that yield the appearance of several self-accommodating variants, then, an optical micro characterization is achieved to focus different microstructures of the alloy in the martensitic state.

Key words: Young's modulus, shear modulus, ultrasonic waves, longitudinal velocities, transverse velocities, non-destructive ultrasonic testing, shape memory alloy.

Corresponding Email: debboub-salima@univ-eltarf.dz

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Antimicrobial activity of mint essential oils

Ouafia LIAMANI[1], Hasna ZEBLAH[2], Lahouaria LABGA[3], Sofia EL HASSAR[2], Fatima BENAZZOUZ[2], Amina KHALDI[1], Mohamed Lamine BENINE[1]

[1]Environmental information synthesis laboratory, Djillali Liabes University. Sidi bel abbes, Algeria
[2] Department of Biology, Faculty of Natural and Life Sciences, Djillali Liabes University. Sidi bel abbes. Algeria
[3]Laboratory of Biotoxicology, University Djillali Liabès Sidi Bel Abbès, Algeria

Abstract

Our work is based mainly on a study of essential oils of mint (Mentha spicata) in the region of Sidi Bel Abbes. Mint, widespread in Algeria, of the family Lamiaceae is an herb native to several therapeutic properties (antiseptic, anti-neuralgic, analgesic ...). The extraction of the aromatic fraction offers new perspectives in aromatherapy. The extraction of essential oils from mint, accomplished by hydrodistillation just after flowering, gave a yield of 0.64% acceptable and may be cost effective on an industrial scale. The antimicrobial activity of the EO was investigated by disc diffusion and broth micro dilution methods. EO was evaluated for their antibacterial activity against 4 microorganisms: Escherichia coli, Staphylococcus aureus, Pseudomona aeruginosa, , Aspergillus niger. The determination results of antibacterial activity by agar disk diffusion method ranged from 5 to 21 mm of the growth inhibition zone. The essential oils and extracts of the plants studied showed interesting antimicrobial activity against all microbial strains tested.

Keywords: Bacterial strains, Mentha Spicata, essential oils, activity Antibacterial

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

ADSORPTION OF PARA-NITROPHENOL ON CYCLODEXTRIN BASED-MATERIAL COATED BY BENTONITE

Cherifa Hakima MEMOU [a], Hanane MAHROUG [b], Sonia BOUMENDIL [c]

[a] Laboratory of Physical and Macromolecular Organic Chemistry, Faculty of Exact Science, chemistry departement Djillali Liabes University, Sidi Bel Abbes 22000, Algeria

[b]Departement of Hydralic, Institute of Science and Technology, University Center of Maghnia, Algeria

[c] Laboratory of Chemistry of Bio and Nano Systems, Faculty of Exact Science, Chemistry Departement Djillali Liabes University, Sidi Bel Abbes 22000, Algeria

Abstract:

sorption of p-nitrophenol from water by bentonite/ poly(4-vinylpyridine-g-(6-o-monotosyl-6-desoxy-β-cyclodextrin)) composite was studied. studies concerning the sorption kinetic and isotherm are presented and discussed. results of adsorption experiments showed that the adsorbent exhibited high sorption capacities toward p-nitrophenol. the adsorption capacity of the bentonite/ poly(4-vinylpyridine-g-(6-o-monotosyl-6-desoxy-β-cyclodextrin)) material increased as the dosage of the material increased. two isotherm equations have been tested in the present study, namely freundlich and langmuir. the characteristic parameters for each isotherm have been determined. the freundlich equation represented the best fit of experimental data than the other isotherm equation.

Key words: cyclodextrin, p-Nitrophenol, clay, sorption, isotherm.

Corresponding Email:

cherifa_h1996@yahoo.fr

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Adsorption Modeling of Various Phenols on Activated Carbon Fibers using Convolutional Neural Network (CNN) and Support Vector Machine with Dragonfly Algorithm

Hakim Bouzemlal[a], *Mohamed Hentabli*[a] , Abdellah Ibrir[a], *Mohamed Kouider Amar*[a], *Ahmed* Chabane[b]

[a]Laboratory of Biomaterials and Transport Phenomena (LBMPT), Faculty of Technology, University Yahia Fares of Médéa 26 000, Médéa, Algeria.

[b] Laboratoire des Matériaux Organiques (LMO), Faculté de Technologie, Département de Génie des Procédés, Université de Bejaia, Bejaia, Algeria

Abstract:

The aim of this study is to develop numerical models utilizing machine learning techniques and cheminformatics for predicting the equilibrium adsorption capacity (qe) of various phenols (including phenol, 2-chlorophenol, 4-chlorophenol, 2,4,6-trichlorophenol, 4-nitrophenol, and 2,4-dinitrophenol) adsorbed by Activated Carbon Fibers (ACF). A dataset comprising 129 data points was compiled from previously published literature. The modeling inputs include temperature (T), equilibrium concentration (Ce), and molecular descriptors aimed at distinguishing between the studied phenols. Prior to modeling, the data underwent preprocessing through statistical analysis to ensure suitability. Results indicate the superior performance of Convolutional Neural Network (CNN) and Support Vector Machine with Dragonfly Algorithm, as evidenced by their determination coefficients close to unity and root mean squared errors close to zero.

Key words: Adsorption, Activated Carbon Fibers, Convolutional Neural Network, Support Vector Machine, Molecular Descriptors.

P-131

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Electronic and optical properties of $Hg_{1-x}Cd_xTe$ ternary alloys

Mohammed El Amine BOULEKBACHE *[,a], Miloud BENCHEHIMA [a,b], Abdelhadi LACHABI[a], Hamza ABID[a]

[a]*Applied Materials Laboratory, Research Center (CFTE), Sidi Bel Abbès Djillali Liabes University, 22000, Algeria*
[b]*Electronic Department University of Sciences and Technology of Oran, Mohamed Boudiaf (USTO), El M'nouar BP 1505, Oran, Algeria*

Abstract:

The motivation of our study is to examine the physical properties of $Hg_{1-x}Cd_xTe$ ternary alloys to explore their usefulness for optoelectronic devices. Structural ,electronic and optical properties of $Hg_{1-x}Cd_xTe$ ternary alloys are investigated via the (FP-LAPW) method within the densityfunctional theory(DFT) [1, 2]. Where, different generalized gradient approximations are used for approximating the exchange-correlation effects. For analyzing electronic and optical properties, the exchange–correlation energy was handled using the Wu-Cohen generalized gradient approximation (WC-GGA) [3] approach and (TB-mBJ) [4] was also used. The optical properties are determined of $Hg_{1-x}Cd_xTe$. In general, our results are in agreement with the available experimental and theoretical data reported in the literature. Based on our obtained results, direct band gaps and optical parameters, both ternaries are very for manufacturing different microelectronic and, optoelectronic devices.

Key words: II-VI semiconductor compounds; Density Functional Theory; Ternary Alloys; optoelectronic properties**;** (TB-m BJ) approach

Corresponding Email: amine-29-med@hotmail.com

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Structural, elastic, thermodynamic and electronic properties of LuX (X = N, Bi and Sb) compounds: first principles calculations

AMERI Mohammed [a], BLAHA Lamia Farah[a], KHATIR Radja[b]

[a]University Djillali Liabbes Sidi Bel Abbes . Physico-Chemiistry Laboratory of Advanced Materials
[b] Laboratory of Electrical Engineering and Materials (LGEM), Oran, 31000, Algeria

Abstract:

The physical properties of LuX (X = N, Bi and Sb) were studied using the ab initio method based on density functional theory DFT using the Generalized Gradient Approximation (GGA) and the of the local spin density to treat the exchange-correlation potential. The structural parameters such as the lattice parameters a0, the volume modulus B, its pressure derivative B' are in good agreement with the expirimentale. The elastic constants were calculated at 0 K. The thermodynamic properties of LuX using Debye's quasi-harmonic model are studied. The temperature and pressure variation of the volume was calculated with gibbs. The calculated results are consistent with other data

Key words: DFT, GGA , GIBBS .

P-133

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Biosynthèse de nanoparticules de ZnO et évaluation de leurs propriétés chimiques et biologiques.

***Kinza Amel BELHADJI*[1], *Mohamed Cherif TERKHI*[1], *Nadia MESSAOUDI*[1], *Fatiha ABASSENE*[1], *Leila BENDAHMENE*[1], *Fatiha ABDELMALEK*[1], *Ahmed ADDOU*[1]**

[1]*Laboratoire des Sciences et Techniques de l'Environnement et de la Valorisation (STEVA), Faculté des sciences et de la technologie, Université de Mostaganem, Algérie.*

Abstract:

L'oxyde de zinc (ZnO) est l'un des matériaux qui offre beaucoup d'avantages, grâce à ses propriétés très intéressantes, peut être synthèse grâce à déférente méthodes : physique, chimique et Biologique … etc. Dans cette étude, des nanoparticules de ZnO, sous forme de poudre ont été synthèses par la méthode verte ont utilisant l'extrait naturel des plantes. Ces nanomatériaux ont été caractérisés par plusieurs techniques : spectroscopies FTIR et la DRX, MEB. Leurs propriétés photo catalytiques sont évaluées par la photo dégradation du colorant méthyle violet sous irradiation solaire. On a enregistré un taux d'élimination de 90% en présence des nanoparticules de ZnO. Les résultats de la capacité d'adsorption ont montré que l'adsorption maximale (15.01 mg/g) du chrome a été observée à la concentration de 0.05 g de NPs d'ZnO. Les résultats montrent aussi que l'adsorption du Cr dépend de la concentration des NPs et non pas du pH. Ces matériaux exercent un pouvoir antimicrobien important contre la majorité des bactéries à savoir *E coli, Staphylococcus aureus et Pseudomonas aeruginosa* responsables des infections urinaires et de la lithiase d'infection. Le comportement antioxydant des nanoparticules de ZnO a été évalué en piégeant les radicaux libres de l'hydrate de 2,2-diphényl-1-picrylhydrazyl (DPPH) en faisant varier la concentration des nanoparticules et l'intervalle de temps individuellement. Nous avons atteint la capacité de piégeage des nanoparticules de ZnO jusqu'à 90 % en 90 min.

Key words: Synthèse verte, Effet photocatalytique, Plantes, ZnO, adsorption, activité antibactérienne, DPPH

Corresponding Email : ***amelkenza@yahoo.fr***

References

[1] J. Suresh, G. Pradheesh, V. Alexramani, M. Sundrarajan, S.I. Hong, Green synthesis and characterization of zinc oxide nanoparticle using insulin plant (Costus pictus D. Don) and investigation of its antimicrobial as well as anticancer activities, Advances in Natural Sciences: Nanoscience and Nanotechnology, 9 (2018) 015008.

[2] Z. Emami-Karvani, P. Chehrazi, Antibacterial activity of ZnO nanoparticle on gram-positive and gram-negative bacteria, African journal of microbiology research, 5 (2011) 1368-1373.

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Isotherme d'adsorption d'un colorant cationique par charbon actif à base de coques de noix

Halima DELALIa, Zohra BAHNESb , Aicha MEDJDOUBc , Khedidja DAHMANId, Mohammed Amin CHEMRAKe,Nawel MOUSSAf,Asmae BENABBOUg , Iman GOUAICHh, , Mostefa BELHAKEMi

[1]Environmental information synthesis laboratory, Djillali Liabes University. Sidi bel abbes, Algeria

[2] Department of Biology, Faculty of Natural and Life Sciences, Djillali Liabes University. Sidi bel abbes. Algeria

[3]Laboratory of Biotoxicology, University Djillali Liabès Sidi Bel Abbès, Algeria

Abstract

Notre étude se concentre sur l'analyse de l'isotherme d'adsorption d'un colorant cationique par les coques de noix. Nous avons initié nos travaux en caractérisant la surface du charbon actif à l'aide d'une analyse infrarouge par transformée de Fourier, révélant la présence de groupements oxygénés en surface. L'étude des facteurs (temps, dose et pH) a révélé que les taux d'élimination optimaux sont obtenus avec un temps de contact adsorbat/adsorbant de 3 heures, une dose de biosorbant de 2 g/L, et une solution de colorant à pH acide. Selon la classification de Giles et Coll., l'adsorption étudiée correspond au type L. Les modèles isothermes de Langmuir et de Redlich Peterson ont montré les meilleures correspondances, avec des coefficients de détermination R^2 supérieurs à 0,99.

Keywords: adsorption ; charbon actif ; colorant cationique.

P-135

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

First Principale calculations of structural,elastic,électronic and magnetic propretiesofAg2BGd fullHeusleralloycomoundsusingGGAandGGA+U: FP-LMTO calculations

Bourahla Asma[a,b], Ameri Mohammed[b,c].

[a]'Laboratory of physical Chemistry of Advenced Materials, University of Djillali Liabes,BP89,22000 Sidi-bel-Abbes ,Algeria
[b] Department: "Materials and Components,Faculty of Physics University of Science and Technology Houari-Boumediene, Algeria
[c] Physics Department,Faculty of Science,University of Sidi-Bel-Abbes,2200, Sidi-Bel-Abbes,Algeria

Abstract:

A series of full-Heusler based on rare earth Ag_2BSmare studied by liner muffin-timorbital FP-LMTO method. Withimgeneralized gradient approximationGGAand GGA+U inthe frame ofdensityfunctionaltheoryDFT.We havestudiedthe structural, elastic, electronicand magnetic properties. We have found that our three compounds are stable in $AlCu_2Mn$ type.

The elastic constants at equilibriumare also determined. We have the bulk and shear modulus(G), young'smodulus(E),poison'sratio (ν),ratio(B/G)andwehavededuced anisotropic parameter (A).

Fromtheparameter'sbehavior,it isinferredthatthesealloysareelastically stableandductile in nature. The magnetic moments of boththe materials in both cubic phases have been calculated.

Keyword: rare earth, DFT, FP-LMTO, GGA, GGA+U, magnetic

Corresponding Email: bourahlaasma92@gmail.com

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Molecular docking and pharmacokinetics studies of a synthesized Schiff base

Manal CHETTIBI[a], Saida SERIDI [b], Marwa BENMABROUK [c].

[a] Manal CHETTIBI' Laboratory of Physical Chemistry, University of 8 Mai 1945, BP 401, Guelma, Algeria
[b] Saida SERIDI' Laboratory of Physical Chemistry, University of 8 Mai 1945, BP 401, Guelma, Algeria
[c] Marwa BENMABROUK' Laboratory of Physical Chemistry, University of 8 Mai 1945, BP 401, Guelma, Algeria

Abstract:
Biochemistry and medicine place a great deal of emphasis on Schiff bases. As such, they are considered promising candidates for the development of drugs such as antibiotics, antivirals, anti-inflammatories, antitumors, and anticancer agents.

A Schiff base ligand, specifically 2-{(*E*)-[(4-hydroxyphenyl) imino] methyl}phenol was successfully synthesized and characterized. The ligand was subjected to molecular docking studies using two different software AutoDock Vina and MOE with a distinct lung cancer receptor, identified by his Protein Data Bank (PDB) code: 1x2j.

The ADME-Tox properties were utilized to evaluate the potential efficacy, safety, and pharmacokinetic profile of the drug candidate. Moreover, the Lipinski's rule was employed to assess the probability of the molecule becoming a viable drug.

Key words: Schiff base, Molecular docking, ADME-Tox.

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Application of the sorption process in the elimination of MB in aqueous solution by Alginate-sepiolite biocomposite beads: adsorption kinetic, and modeling

Kheira Chinoune [a], Amel Mekki [b,c], Amina Sardi [f], Mohammed Hachemaoui [b,g], Adel Mokhtar [b,e] , Bouhadjar Boukoussa [b, d]

Abstract

This work is based on the preparation of biocomposite beads Alginate-Sepiolite using a simple preparation method. A series of materials was prepared by varying only the mass of the sepiolite in the biocomposite beads (mass of the sepiolite is varied between 0.5-1.5 g in the reaction mixture). The obtained biocomposites were characterized by XRD, FTIR, TGA, XRF, SEM, and EDX and then tested as adsorbents for the removal of Methylene Blue MB dye in an aqueous solution. To study the adsorption behavior of MB dye on biocomposites, several parameters affecting MB adsorption were investigated and discussed. The results obtained showed that the ALG-Sep composite hydrogels were well formed, and their properties were improved depending on the sepiolite content used. The kinetics and modeling results show that the adsorption process follows first-order kinetics, and the Langmuir model. It was found that the adsorption capacity of MB dye increased with the increase of sepiolite in the composite beads, and adsorption was carried out in the following order ALG-Sep(1.5) > ALG-Sep(1) > ALG-Sep(0.5). The maximum absorption capacity of MB dye on ALG-Sep(1.5) was qmax = 55.49 mg.g-1. Among the advantages of this biocomposite is that it is prepared from natural and non-toxic sources, and it is easily separable after adsorption, which makes it an excellent candidate for the elimination of organic pollutants in polluted waters.

Keywords: MB dye adsorption, sepiolite, alginate, composite beads, kinetic, modeling.

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Solubility of asphaltenes in two polar solvents .

Ghalem Ikram[1], Daaou Mortada[2] , Bounaceur Boumediene[1] ,Naamoun Karima[1]

[1]Departement of chemistry, laboratory of physical chemistry and macromolecules, University of Oran 1-Ahmed Ben Bella, P.O. Box 1524, Oran,31005, Algeria

[2]Departement of industrial chemistry laboratory of organic synthesis, physical chemistry, biomolecules and environment, University of Sciences and Technology of Oran, Post Office Box 1505, 31036 El-M'naouer, Algeria.

Abstract

The aim of this work is to explore the flocculation behavior between asphaltenes (extracted from a deposit recovered from a Hassi-Messaoud oil well) in solution with two solvents (toluene and DCE) and n-heptane as the flocculating medium using UV-VIS spectrophotometer. Deriving the Hildebrand solubility parameters for the flocculated asphaltenic fractions is done with the Donnagio method using Flory-Huggins theory.

Keywords: Asphaltenes, Solubility, Flocculation.

P-139

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

O-LiDAR Performance Analysis for different Jerlov Water types

KANDOUCI Chahinaz, BOUZIANI Merahi

Telecommunications and Digital Signal Processing Laboratory, Faculty of Electrical Engineering Sidi Bel Abbes , Algeria

Abstract:

Oceanic Light Detection and Ranging (O-LiDAR) represents a significant remote sensing apparatus utilized for the assessment of near-coastal water depth and the exploration of optical attributes within aquatic environments [1]. The proliferation of LiDAR commercialization has spurred heightened global inquiry into the theoretical underpinnings governing the transmission properties of LiDAR in underwater settings.

In optical oceanography, Jerlov categorized waters into oceanic and coastal types based on their chlorophyll concentration. The latter directly affects the water's particles sizes and consequently the scattering and absorption effects on any light beam propagation underwater [2],[3]. In order to overcome those drawbacks, we propose to translate the benefits of Optical Code Division Multiple Acces (OCDMA, more traditionally implemented in optical fibers systems) in UWOC systems by using two dimensional wavelength hopping / time spreading (WH/TS) codes to generate and detect the O-Lidar impulsions[1].

Key words: O-Lidar, OCDMA, Jerlov water types.

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Numerical analysis of residual stresses and warpage of thin-film coated silicon wafers

Amer MECELLEM [1], Douaa KHELLADI[1], Sofiane BELHENINI[1]

Mechanical engineering, BELHADJ BOUCHAIB University, AIN TEMOUCHENT, ALGERIA

Abstract:

Thermal cycling testing is a time-consuming and expensive endeavor due to the specialized equipment and electrical setups required. For instance, a single 1000-cycle[19] test can take up to 21 days to complete. Moreover, multiple tests are often necessary to ensure repeatable results, further escalating the associated costs. These additional expenses, coupled with production costs, can pose significant challenges to engineers tasked with developing new electronic components. Additionally, identifying failure modes is a complex and costly undertaking, necessitating the use of numerical methods to estimate the stresses and deformations induced by the testing process. The chosen method for this analysis is finite element modeling (FEM), FEM is a well-established numerical technique widely used to assess the mechanical and thermomechanical reliability of electronic devices. It involves computer simulation of thermal cycling tests, enabling the determination of stress, strain, and displacement fields within each component. This investigation focuses on a numerical simulation of the thermal cycle of a physical component, i.e. the integration of a WL-CSP (Wafer-Level Chip Scale Packaging) microcomponent onto a standard printed circuit board (PCB). A series of simulations of the thermal cycle test are performed using a research version of the commercial software Abaqus. [1]

Key words: Silicon wafers,residual stresses,Thermal cycling testing, Thin Films, Abaqus, WL-CSP, Finite element modeling, PCB

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Physicochemical and biological characterization of residual discharges from the National Electronic Industries Company of Sidi Bel Abbes and risk assessment.

El Badaoui Naima[a]., Rachedi Mohamed[b]

[a]·Laboratory of Molecular Microbiology and Proteomics and Health, Faculty of Nature and Life Sciences, Djilali Liabes University of Sidi Bel Abbes, 22000, Algeria;

[b]Chef de département Epuration et Assainisseement, ENIE/Spa, Entreprise Nationale des Industries Electroniques (E.N.I.E.), *Sidi Bel Abbes, 22000, Algérie.*

Abstract: The National Electronic Industries Company of Sidi Bel Abbes (ENIE of SBA) is equipped with a wastewater and sludge purification plant to reduce the pollutant load in order to reuse them and avoid the phenomenon of eutrophication and the contamination of groundwater, because the excess is discharged into Oued Mekerra. The aims of this work is the physicochemical and biological quality control of the treated water and sludge from the ENIE, in order to evaluate the effectiveness of the treatment plant and assess the risks. The results obtained show that the wastewater is loaded with NO_3-, Ca^{+2} Mg^{+2}, NA Cl, Cl^-, So_4-2. While the heavy metals Br, Fe, Cu^{2+}, CN^-, F are present in small quantities but comply with standards, with the exception of Cr^{+6}. The biological analysis showed that the BOD_5 of the purified water (90 mg/l) was not compliant from a bacteriological point of view. On the other hand, the COD_5 (150 mg/l) does not comply with the standard for sludge, which promotes microbial development and an increase in the concentration of nitrites, sulfides and ferrous irons in solution. In conclusion, the wastewater analyzed can have a harmful effect after its discharge into Oued Mekerra or after its reuse. As well as the stored sludge can cause atmospheric pollution. View these results we deduce that those responsible for the ENIE company must improve the installations within the wastewater treatment plant (bleaching or sterilization devices and installation of filters), as well as carry out techniques for depolluting the sludge stored for avoid environmental risks.

Key words: ENIE of SBA, wastewater, sludge, quality, assess the risks

Corresponding Email: elbadaoui.naima@gmail.com

References

[1] Journal officiel de la République algérienne nº 46, 14 juillet 1993, Décret exécutif n° 93-160 du 10 juillet 1993 réglementant les rejets d'effluents liquides industriels. 9 p.

[2] Rodier J., Legube B., Merlet N. 2016. L'analyse de l'eau, Eaux naturelles, eaux résiduaires, eau de mer. *Ed*. Technique et ingénierie, Dunod, 1824 p.

P-142

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Ab-initio Investigation of the Structural and Dynamical Stability of Ni_2MnSi Full-Heusler Alloy.

L. Beldi, H. Bendaoud, and B. Bouhafs
Laboratoire de Modélisation et Simulation en Sciences des Matériaux, Département de Physique, Université Djillali Liabès de Sidi Bel-Abbès, Sidi Bel-Abbès, 22000, Algeria.

ABSTRACT:

Heusler alloys [1] have been attracting continuously growing interest due to their diverse properties for spintronics. The full-Heusler alloy Mn_2VAl was the first one proposed to be a half-metallic ferromagnet (HMF) and has been studied in detail both experimentally and theoretically [2]. Ni-based full-Heusler alloys have attracted research attention because they exhibit shape memory effect when subjected to external magnetic field and temperature [3,4], particularly the Ni_2MnSi full-Heusler alloy.
In this work, first-principles calculations were carried out to study the structural and magnetic stability of the cubic (Cu_2MnAl ($Fm\bar{3}m$), Hg_2CuTi ($F\bar{4}3m$)), and tetragonal ($I4/mmm$, $I\bar{4}m2$) phases of Ni_2MnSi full-Heusler alloy. The structural, cohesive, elastic, mechanical, phonon, thermodynamic, magnetic, and electronic properties were determined.

The results show that Ni_2MnSi alloy is stable in the tetragonal *I*4/*mmm* phase, with a metallic ferromagnetic character. The phonon dynamics analysis indicates that the cubic Cu_2MnAl and the two tetragonal ($I4/mmm$, $I\bar{4}m2$) phases are dynamically stable, unlike the cubic Hg_2CuTi phase which is dynamically unstable due to the presence of imaginary modes in the phonon dispersion. The observed magnetism in this alloy is mainly due to the 3*d* states of Mn and Ni atoms.

Key words: Density functional theory; Phase stability; Full-Heusler; Ferromagnatism.

Corresponding Email: l_beldi@yahoo.fr

References

[1] Z. Wen, H. Hou, J. Tian, Y. Zhao, H. Li, P. Han, *Intermetallics* 92, **2018**, 15–19
[2] A.T. Zayak, W.A. Adeagbo, P. Entel, K.M. Rabe, *Appl. Phys. Lett.* 88, **2006**, 111903.
[3] R. De Groot, F. Mueller, P. Van Engen and K. Buschow, *Phys. Rev. Lett.* 50, **1983**, 2024.
[4] S. Ishida, S. Asano and J. Ishida, *J. Phys. Soc. Jap.* 53, **1984**, 2718.

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Development of microparticles based of polysaccharides as novel drug release systems

Mohammed DELLALI [1] , *Kheira ZANOUNE* [1] ,*Camelia Elena IURCIUC (TINCU)*[2] *and Marcel POPA*[2,3]

[1] *Faculty of Technology , Hassiba Benbouali University of Chlef, Algeria,*
[2] *"Gheorghe Asachi" Technical University of Iasi, Romania,*
[3]*Academy of Romanian Scientists, Splaiul Independentei 54, Bucuresti, Romania*
***Corresponding author e-mail**: dellali_m@yahoo.fr*

Abstract

Curcumin is an active ingredient obtained from tumeric rhizomes, *Curcuma longa*, having a strong antioxidant, anti-inflammatory, antimicrobial and anti-tumor effect [1]. There been reported beneficial effects of using curcumin in the treatment of diseases such as cystic fibrosis, intestinal diseases, Alzheimer, diabetes and metabolic syndromes. The pharmacological effects of the curcumin are limited due to the low solubility in water and is rapidly metabolized and eliminated regardless of the route of administration, which leads to a very low bioavailability. These disadvantages can be overcome by the curmin inclusion in the polymeric matrices [2].

The polysaccharides have been shown to be effective in the immobilization of various active ingredients since they are biodegradable, non-toxic and can be used in the preparation of various supports for controlled release of the active ingredients in a target site in the body [3]. The curcumin encapsulation was performed using the particles based on polyelectrolyte complexes between the polysaccharides with different ionic character. The type consists of microparticles based on chitosan with curcumin immobilized included in a protein (lactalbumin) spherical matrix ionically cross-linked with magnesium acetate obtained by an extrusion process in the aqueous mediums containing different magnesium acetate concentrations. The particles ability to swell in different environments and the release kinetics study was evaluated at pH= 7.4 and pH 3. The values of the swelling degree are higher in the slightly basic medium. The release kinetics studies were carried out in the presence of Tween 80 over a longer period of time of 6000 minutes. The release curves are typical for the systems polymer-active principle with release caused by the diffusion. The release efficiency increases with decreasing of the cross-linking degree and when in the polymer mixture composition is an amount of protein that determine a higher porosity in the particles.

Keywords: Curcumin ; Particles ; polysaccharide ; Immobilization, release system.

References

1. K.I. Priyadarsini, Photophysics. *J. Photochem. Photobiol. C,* **2009**, 10, 81.
2. K. Priyadarsini. *Molecules*, **2014**, 19, 20091.
3. M. Al-Remawi. *J. Excipients and Food Chem.*,**2015**, 6, 34.

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Title: Preparation of a new composite by ultrasonic method (catalytic reduction application)

Saadia Belkiour [1], Farouk Zaoui [1,2], Bouchra Elhadjdaouadji [1], Amel Iles [3], Fatima Zohra Sebba [1]

[1]chimie, Laboratoire de chimie physique macromoléculaire University Ahmed Ben Bella Oran1, B.P 1524 El-Menaouer , 31000, Oran, Algeria. .
[2]chimie, Centre universitaire ElCherif Bouchoucha, Aflou B.P 306, Laghouat,Algeria.
[3] chimie, Laboratoire de synthèse organique appliqué (LSOA), University Ahmed Ben Bella Oran1, 31000, Oran, Algeria.

Abstract:

This work concerns the preparation of a new composite material based on poly(Glycidyl methacrylate), Ru/TiO2 and Fe3O4 using ultrasound treatment. Several composites were prepared by varying the percentage of Ru/TiO2 and Fe3O4. Then, they were applied as catalysts for the reduction of several organic pollutants. 4-Nitrophenol (4- NPh), Methylene blue (MB) and Orange G (OG) were used as a model to study the photocatalytic reduction process in the presence of NaBH4 at room temperature. The obtained photocatalysts were characterized by different methods such as XRD, FTIR, XPS, SEM, EDX, TEM, STEM, TGA, ultraviolet–visible (UV–vis) spectroscopy and Zeta potential measurements. The results showed that the use of ultrasound gave a good dispersion of all species into the polymeric matrix. These solids have shown good activity via the photocatalytic reduction of organic pollutants. The best performance was obtained for the photocatalyst having the higher content of metal NPs "CP(30)". The rate constant Kapp of composite CP(30) towards catalytic reduction of MB, OG and 4-NPh reached a high level up to 0.55 min□ 1, 0.241 min□ 1 and 0.3 min□ 1, respectively. Finally, the recyclability of the photocatalyst CP(30) was also

evaluated. The results showed that the performance of this photocatalyst was satisfactory during its reuse.

Key words:
Poly(GMA) ,Ru nanoparticles, TiO2, Fe3O4 ,Catalytic reduction

Corresponding Email: Belkioursaadia96@gmail.com

P-145

ICMSE'2024

The 3rd Edition of the international conference on materials science and engineering and their impact on the environment

Thermal vibration analysis of FGM Structures

Abdelkader SAFA[a], Lazreg HADJI [b], GUERMIT Chami mohamed Bilal [c], Mohamed BOURAADA[d],

[a]Department of Civil Engineering and public works, Ahmed Zabana University, Relizane 48000, Algeria.
[b] Department of Civil Engineering, Ibn Khaldoun University, BP 78 Zaaroura, 14000, Tiaret, Algeria.
[c] Department of Civil Engineering, Mouloud Maamri University, 15000, Tizi ouzou, Algeria.
[d]Material and Hydrology Laboratory, University Djilali Liebes, Sidi Bel Abbes,22000, Algeria.

Abstract:

An efficient shear deformation beam theory is developed for thermo-elastic vibration of FGM beams. The theory accounts for parabolic distribution of the transverse shear strains and satisfies the zero traction boundary conditions on the on the surfaces of the beam without using shear correction factors. The material properties of the FGM beam are assumed to be temperature dependent, and change gradually in the thickness direction. Three cases of temperature distribution in the form of uniformity, linearity, and nonlinearity are considered through the beam thickness. Based on the present refined beam theory, the equations of motion are derived from Hamilton's principle. The closed-form solutions of functionally graded beams are obtained using Navier solution. Numerical results are presented to investigate the effects of temperature distributions, material parameters, thermal moments and slenderness ratios on the natural frequencies. The accuracy of the present solutions is verified by comparing the obtained results with the existing solutions.

Key words: FGM beams, Hamilton's principle, thermal moments, Navier solution, natural frequencies.

Corresponding Email:

abdelkader.safa@univ-relizane.dz

References

P-146

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Title: The mechanical behavior of polymer biomaterials.

Fatma REMIL [a,1], Ali MERDJI [a,2], Noureddine Abdelkader DELLA [a,3],

[a] Department of Mechanical Engineering, University of Mascara, Algeria.

Abstract:

Polymer biomaterials play a crucial role in various biomedical applications, ranging from tissue engineering to drug delivery systems. Understanding their mechanical behavior is essential for designing effective and durable biomedical devices and implants. This PhD research aims to investigate the mechanical properties of polymer biomaterials through experimental characterization and computational modeling techniques. The study will explore the influence of material composition, processing methods, and environmental factors on the mechanical performance of polymer biomaterials. Additionally, advanced techniques such as finite element analysis and molecular dynamics simulations will be employed to elucidate the underlying mechanisms governing their mechanical behavior at different length scales. The outcomes of this research will contribute to the development of improved polymer biomaterials with tailored mechanical properties, enhancing their suitability for diverse biomedical applications and ultimately advancing the field of biomaterials science and engineering.

Key words: Polymer biomaterial, Mechanical behavior, Mechanical properties, Finit element analysis, Numerical model.

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Microscopic study of the effect of desert environmental factors on the materials that make up solar panels

Nadir Hachemi*[1], El fahem Sakher[1], Messaouda Chaib [1] Façal Baira [2] Rachid Tigrine [1]

1 Department Of Material Science, Laboratory Of Energy Environment And Information(LEESI) Adrar, Algeria

2 Department of Sciences and technology, Faculty of technology, University of Batna 2, Alleys 53,Constantine Avenue. Fésdis, Batna 05078, Algeria

Abstract:

Deploying solar panels in desert areas exposes them to harsh environmental conditions that can accelerate material degradation and reduce performance over time. We performed microscopic studies to learn how high temperatures, airborne particles, and extreme UV radiation affect common solar panel materials at the micro level. Advanced analytical techniques such as scanning electron microscopy, X-ray spectroscopy, and infrared spectroscopy have revealed specific degradation mechanisms. For example, silicon photovoltaics showed micro-cracks and delamination, transparent conductive oxides showed increased surface roughness and chemical changes, polymer capsules suffered from photo-oxidation and de-crosslinking, while anti-reflective coatings were susceptible to abrasion by wind-borne sand particles. These microscopic evaluations provide valuable insights into material failure modes, guiding the development of more durable solar panel components designed to withstand the harsh desert environment.

Key words: photovoltaics , microscopy X-ray spectroscopy, material degradation .

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Comparative study of the environment in metal complexes. DFT and TD-DFT study

Sonia BOUMENDIL [a], Cherifa Hakima MEMOU [b]

[a]Chemistry Department, Laboratory of Chemistry of Bio and Nano Systems, Faculty of Exact Sciences, Djillali Liabes University, Sidi Bel Abbes, Algeria
[b]Chemistry Department, Laboratory of Physical and Macromolecular Organic Chemistry, Faculty of Exact Sciences, Djillali Liabes University, Sidi Bel Abbes, Algeria

Abstract:

Solvent-solute interactions can change the geometry, the electronic structure and the dipole moment of a solute, but also many other properties. Among them, the UV/Vis absorption spectra of chemical compounds are influenced by the surrounding and vary with the polarity of the medium: solvents can bring about a change in the position, intensity, and shape of absorption bands, this is a solvatochromism phenomenon [1]. A large majority of experimental data being measured in solvated phase, it is mandatory to take these effects into account.

Theoretical chemistry methods are very powerful tools to understand these properties. For this reason, this study will focus on the integration of solvent effects in the reproduction of UV-Vis data, more precisely in the framework of TD-DFT computations.

The study of solvent effects may be classified in two major descriptions. The explicit model, it is to introduce around the chemical system explicit solvent molecules. The main advantage of this description is the inclusion of solvent-solute interactions such as hydrogen bonds. It also helps to know the structure of the different layers of solvation. The major disadvantage of this model is the very important computation time. On the contrary, the implicit model is more rapid due to the lower number of electrons to take into account: the

chemical system is here immersed in a dielectric continuum. The solute and the solvent are separated with a cavity whose size and geometry are defined by the model. The most important disadvantage is to ignore some specific short-range effects. In this study the "Polarizable Continuum Model" (PCM) will be used.

Between these two approaches lies some intermediates descriptions referenced as microsolvation models where a small number of solvent molecules are added around the molecule of interest, the solvent bulk being described by a continuum model.

These approaches will be illustrated on the specific case of the complex between caffeic acid and aluminum (III) cation and it will be shown that the dual role of solvent molecules in this case (both solvent and ligand) require to use a microsolvation model.

Key words: Caffeic acid, TD-DFT, solvent effect, UV-Vis spectra.

Corresponding Email : bouson1780@gmail.com

References

[1] Andrzej Eilmes, Theor Chem Acc, 133 (2014) 1538

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Title: Optimization of Tin Bath Parameters to Enhance Efficiency in 3mm Thin Glass Production.

Meftah souad[a], Djebli abdelkader[b].

[a]Faculty of Science and Technology, University of Mascara, Algeria
[b]Faculty of Science and Technology, University of Mascara, Algeria

Abstract:

This work explores the optimization of performance at Mediterranean Float Glass (MFG), focusing on the influence of tin bath parameters on the thickness of 3 mm clear glass and analyzing production losses. It delves into various tin bath components, such as Top Rolls, which affect glass thickness, and coolers, which impact ribbon temperature homogeneity. The study identifies and addresses production inefficiencies, aiming to increase efficiency and potentially save millions of dinars annually.

Key words: Float glass, tin bath, yield optimization, Top Roll.

Corresponding Email:
souad.meftah@univ-mascara.dz

References

[1] Internal documentation of the MFG factory (CLFG: China Luoyang Float Glass): unit of float glass production.

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Optimization of adsorption capacity: Application of mathematical modeling

Abdelkarim Brahimi[a], Nabila Boucherit[b], Mohamed Laid Yahiaoui[a] , Mohamed Messaoudi[a] and Fayçal Rebhi[a]

[a]Nuclear Research Center of Birine (CRNB), COMENA, BP180 Ain Oussera , Djelfa, Algeria.
[b]Department Sciences of material, Faculty of Sciences, University of Medea, urban pole, Medea (26000) Algeria

Abstract

In this work, a mathematical model that can predict the maximum adsorption capacities of Cu+2 ions was constructed using the results of the parametric study. Various characterization and analysis methods were used to characterize the adsorbent in the initial step, in the second step, adsorption in batch mode results were used to conduct studies such as: parametric, kinetic, and thermodynamic. Optimizing the experimental data obtained in the parametric study was the goal of this work, with the aim of achieving maximum adsorption capacities and saving time. Various experiments were carried out for the purpose of statistical mathematical modeling, to predict the response and accuracy of the model, we used a multiple regression approach with second degree polynomial terms and interaction terms. The independent parameters selected were: the dose of the adsorbent (X1, g/l), the initial concentration of the Cu2+ ion (X2, mg/l) and the temperature of the solution (X3, K). The adsorption capacity of Cu2+ ions (Qe, mg/g) is retained as a response. The formula for the retention capacity Qe was a function of the variables X1, X2, and X3. The calculated coefficient of determination R2 is 0.991. This high value indicates that the mathematical model was able to explain 99.1% of the variance observed in the adsorption capacity of Cu2+. It is an indicator of the high precision and relevance of the model. the optimal regions of the adsorption capacity revealed that the maximum adsorption capacities were observed in the region with low concentration of the adsorbent and high concentration of Cu2+ ions, and under ambient temperature.

P-151

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Title: Structural, elastic, electronic, and optic study of the anti-perovskite Rb_3BrO

Fatiha SAADAOUI*[a] , Nadir CHAMI[b] ,Hayat HOCINE [a] , Fatima Zohra DRISS-KHODJA [a] , Halima HAMADA [a] , Mohammed DRISS-KHODJA

[a] Laboratoire des Etudes Physico-Chimiques, Université de Saïda, 20000 Saïda, Algérie

[b] Departments of Electronics, Faculty of Technology, University of Saïda Dr. Tahar Moulay, 20000 Saida, Algeria

Abstract:

In this work, the structural, elastic, electronic, and optic properties of the anti-perovskites Rb_3BrO compounds have been investigated using the full-potential linearised augmented plane waves (FP-LAPW) method based on the density functional theory (DFT) implemented in the code wien2k. The analysis of the structural and elastic properties of Rb3BrO were performed with mean of the generalized gradient potential (GGA-PBE, GGA-PBEsol) and the local density approximations(LDA) while the electronic, and optical properties have been performed using the GGA-PBEsol approximation. The obtained results of the lattice parameters are in good agreement with the available experimental data. On the other hand, the material is a narrow band-gap semiconductor of 0.41 eV.

Key words: Structural, GGA-PBEsol, Elastic properties, Rb_3BrO

Corresponding Email:

saadaouifatiha@yahoo.fr

References

[7] S. Sitta, K. Hippler, 19 Vogt, H. Sabrowsky, Z. anorg. allg. Chem. 597 (1991) 197

[8] Yinchang Zhao, Chao Lian,Shuming Zeng, Zhenhong Dai, Sheng Meng and Jun Ni PHYSICAL REVIEW B101, 184303 (2020)

P-152

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Le rôle efficace des matériaux à changement de phase (MCPs) dans la résolution de problèmes thermiques anciens *Résumé d'une étude approfondie*

Rachid Djeffal[a,b], Zakaria Triki[c], Abir Abboud[c], Sidi Mohammed El AmineBekkouche[a], Laib dit Leksir Y[d,b], Farh Hichem[d,b]

[a] Unité de Recherche Appliquée en Energies Renouvelables (URAER) Centre de Développement des Energies Renouvelables (CDER), Ghardaïa 47133, Algeria
[b] Laboratoire des Composants Actifs et Matériaux (LCAM), université LARBI BEN M'HIDI -Oum El Bouaghi. Bon courage
[c] CountryLaboratory of Biomaterials and Transport Phenomena, University of Medea, Medea 26000, Algeria
[d] Faculté des Sciences et des Sciences Appliquées, université Larbi Ben Mhidi, Oum el Bouaghi

Abstract:

Les rapports environnementaux de ces dernières années indiquent un changement climatique important, résultant des émissions de dioxyde de carbone résultant d'une consommation excessive d'énergie, en particulier de combustibles fossiles. Dans le même temps, l'approvisionnement en ces sources d'énergie est devenu moins fiable. Pour faire face à ces énormes difficultés, nous devons adopter de nouvelles stratégies visant à rationaliser la consommation d'énergie et à la réduire en nous tournant vers d'autres sources propres et respectueuses de l'environnement, telles que les énergies renouvelables et en améliorant l'efficacité énergétique. L'un des meilleurs moyens de réduire la consommation d'énergie consiste à utiliser des systèmes utilisant des matériaux à changement de phase solide-liquide (MCP) en raison de leur potentiel thermique.

Dans ce résumé, nous avons introduit la matière à changement de phase dans plusieurs modèles qui consomment de l'énergie et provoquent des catastrophes environnementales, tels que les bâtiments, les réfrigérateurs et les chauffe-eau sanitaire. Les résultats obtenus sont très encourageants. Par exemple, dans les logements, nous pouvons réduire plus de 65.9% en ce qui concerne la consommation des bâtiments. De même, pour le réfrigérateur, nous avons

obtenu ce qui représente 12.88%, et la même chose s'applique aux chauffe-eau, où le pourcentage est dépassé 47.42%.

Key words: changement climatique, combustibles fossiles, l'efficacité énergétique, MCP

Corresponding Email: djeffalrachid78@gmail.com

References

[1] Rachid. Djeffal, Cherier MK, Bekkouche. S. M. A, Zohir Younsi, Hamdani M, Saleh Al-Saadi, Concept development and experimentation of a Phase Change Material (PCM) enhanced domestic hot water, Journal of Energy Storage 51(2022) 104400, https://doi.org/10.1016/j.est.2022.104400.

[2] Rachid. Djeffal, S.M.A. Bekkouche, M. Samai, Z. Younsi, R. Mihoub, A. Benkhelifa, effect of Phase Change Material eutectic plates on the electric consumption of a designed refrigeration system, Instrumentation Mesure Métrologie, 19 (1), 2020, 1-8. https://doi.org/10.18280/i2m.190101.

[3] Sidi Mohammed El Amine Bekkouche, Rachid. Djeffal, Mohamed Kamal Cherier, Maamar Hamdani, Zohir Younsi, Saleh Al-Saadi and Mohamed Zaiani. Experimental Performance and Cost-Effectiveness of a Combined Heating System under Saharan Climate. Buildings 2023, 13, 635. https://doi.org/10.3390/.

P-153

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Simulation Study of Semiconductor Perovskite $CsGeCl_3$ for Future Solar Cells Applications

Dhilal ALOUANI [a, *], Samir CHAREF[b]

[a] Study and Research of Condensed States (LEREC) Laboratory, Faculty of Sciences, Department of Physics, Badji Mokhtar University-Annaba, 2300 Annaba, Algeria.
[b] Elaboration and characterization Physical Mechanics and Metallurgical of Materials (ECP3M) Laboratory, Abdelhamid Ibn Badis University-Mostaganem, 27000 Mostaganem, Algeria.

Abstract:

Semiconductor perovskite materials has given interest as a potential thermoelectric material due to its large thermopower. In our study the calculation of different properties of $CsGeCl_3$ are investigate by using First Principal calculations applying the Full-Potential Linearized Augmented Plane Waves (FP-LAPW) method based on Functional Density Theory (DFT) implemented in Wien2k code. The equilibrium lattice parameter of $CsGeCl_3$ is calculated and found to be 5.236 Aº. Modified Beck-Johnson (mBJ-GGA) potential Approximation was used to describe the band structure more accurately, the studied compound ($CsGeCl_3$) exhibits a semiconductor characters with direct bandgap at the R-point in the reciprocal lattice space which is equal to 1.561 eV. Moreover, this compound appears to have higher optical absorption and conductivity, the broad absorption range that corresponds to the visible to ultraviolet energy values shows the utility of this compound for various optoelectronic devices operating in this spectral range. Our result revel that this material can find certain applications in the optoelectronic devices owning to their suitable energy bandgap. Also, could be used for photovoltaic applications.

Key words: Perovskite, $CsGeCl_3$, Solar Cells, Optoelectronic, DFT Method, Wien2k.

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Differential immunochemical characterization of monoclonal antibody directed against the beta casein and its proteolysis products by the plasmin

BELKESSAM Yamina(1), CHARIF Khadidja(2), MEZIANI Samira(1)

(1) Biotoxicologie Laboratory, Department of Biology, Faculty of Natural Sciences and Life, University of Djilali Liabes, Sidi Bel Abbes.
(2) Laboratory of materials and catalysis, Faculty of Exact Sciences, Djillali Liabes University, Sidi Bel Abbes, Algeria.

Abstract

Milk is extremely complex both by its multiphasic physical nature and by the diversity of its molecular constituents whether they are its protein particularly. Caseins (CN), represents of the major protein fraction of this dairy undergoes preferential degradation from proteolysis by plasmin activities in Beta-casein (β-CN) with entrainment of gamma casein (γ-CN) and proteose-peptones. In this work aims to study the β-CN antigenicity and its degradation products in order to develop a milk quality indicator based on the determination of the degree of casein proteolysis. A approach consists in producing and characterizing monoclonal antibodies making it possible to differentiate β-CN from its fragments degraded by plasmin. Immunization and fusion in mice with whole caseins followed by pre-selection of hybrids or clones by use of the indirect ELISA technique and finally determination of affinity constants (Ka) of monoclonal antibody. Interaction between the antibody and the target protein that can be easily monitored by immunoassays such as ELISA. Most of the supernatants studied react better with the degradation products than with the native protein, with each antigen and selected these that recognize strongly the three antigens and those recognizing preferentially either β-CN, either β-5P(f1-105/7), either β-CN(f106-209), (f108-209). Finally, it emerges from these results that the SNC46 and 80 have the best discriminating character. They react exclusively with the C-terminal products of β-CN in immunoblotting as well as by calculation of affinity constants. For the C-terminal fragments against β-CN 1, the SNC25 and 35 also exhibit pronounced reactivity, a weak reactivity observed against the N-terminal fragments of β-CN, in ELISA and in Immunoblot. Monoclonal antibodies will make an important contribution to the study of functional proteins.

Keywords: Milk, Beta-Caseins, Anticorp, monoclonal, ELISA.

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

BIBLIOGRAPHIC REVIEW ON THE VARIOUS METHODS AND TECHNIQUES OF PHYTOTECHNOLOGY

HELLAL Tijania[a], AYACHE Abbassia[b]

[a]HELLAL Tijania' Department of Environmental Sciences, Djillali Liabes university - SNV, Sidi Bel Abbes Algeria. Physico Chemistry Laboratory of advanced Materials (LPCMA)
[b]AYACHE Abbassia' Department of Environmental Sciences, Djillali Liabes university - SNV, Sidi Bel Abbes Algeria.

Abstract:

Over the last twenty years, biodegradation mechanisms have been greatly developed for the protection of the environment. awareness of the danger of the accumulation of domestic pollution (detergents). , industrial and agricultural on the environment and human health has become a major issue in our society. Technologies based on microorganisms, fungi, various plants called bioremediation are used to clean contaminated sites, it is based on several processes such as phytoremediation their techniques are effective, ecological and economical. Phytoremediation is a technology based on the use of green plants to remove, transport, deactivate or destroy harmful environmental pollutants such as heavy metals, radionuclides and hydrocarbons. These plant-based techniques offer several advantages over traditional methods.

Key words: phytotechnology, depollution, remediation, phytoremediation, methods, techniques.

Corresponding Email: tijania.hellal@gmail.com

References

[1] Pierre ROGER et Vincent JACQ, 2000. Introduction à la bioremédiation des sols, des eaux et de l'air. Université de Provence AIX-Marseille 1 E.S.G.B.M.A - E.S.I.L. Luminy

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Optimizing Performance of Perovskite Solar Cells Based on triple cation Perovskite solar cell through SCAPS-1D Device Simulation

Mohammed Cherif Ramdani [a], Khadidja Rahmoun [b], Wissem Benaissa[c] and Katir Ziouche[d]

a Unité de Recherche Matériaux et Energies Renouvelables URMER, University of Tlemcen, Abou Bekr Belkaid, BP 119, Tlemcen13000, Algeria.
b IEMN (Institute of Electronics Microelectronics and Nanotechnology), CNRS-IEMN, University of Lille, France

Abstract:

Triple cation ($Cs_x(MA_{0.17}FA_{0.83})_{1-x}Pb(I_{0.83}Br_{0.17})_3$) perovskites have gained significant attention due to their remarkable stability and photovoltaic performance. This study proposes and theoretically optimizes an efficient perovskite solar cell with a CuO/($Cs_x(MA_{0.17}FA_{0.83})_{1-x}Pb(I_{0.83}Br_{0.17})_3$ (CsFAMA)/ CdS structure using the solar cell simulator capacitance software (SCAPS-1D). The optimization process focuses on parameters such as absorber layer thickness, doping density, defect density, bandgap, as well as electron and hole transport layer (ETL and HTL) properties. The results indicate that optimizing the absorber layer thickness and doping density significantly improves device efficiency, while the ETL and HTL parameters have a minor influence. Furthermore, the impact of operation temperature on device performance is discussed. The solar cell simulation yielded the following values: power conversion efficiency (PCE) = 25.13%, fill factor (FF) = 22.16%, short circuit current density (J_{sc}) = 30.65 mA/cm^2, and open-circuit voltage (V_{oc}) = 3.3 V. These results are compared to previously reported values obtained at specific conditions: doping density of 10^{13} cm^{-3}, absorber layer thickness of 0.1 µm, and temperature of 250 K.

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Simulation study of chalcogenide perovskite (BaZrS3) solar cell by SCAPS-1D

Benaissa Wissem [*] *, Rahmoun Khadidja* [2] *,Cheknane Ali* [3] *, Ramdani Mohammed Cherif* [4]

1,2,4 Unité de Recherche Matériaux et Energies Renouvelables URMER, Université de

Tlemcen, Abou Bekr Belkaid, BP 119, Tlemcen13000, Algérie.

3 Laboratoire des Semiconducteurs et Matériaux Fonctionnels, Université Amar Telidji de Laghouat, BP37G, Laghouat 03000, Algérie.

Abstract:

Chalcogenide perovskites, which are incredibly durable, widely available on Earth, and safe, have drawn a lot of interest recently as possible candidates for a variety of energy conversion applications. In this theoretical investigation, BaZrS3, an inorganic, non-toxic chalcogenide perovskite, is used as the active layer in perovskite based sollar cell, together with TiO2 ETL and the Kesterite CZTS as HTL. This basic cell design may be beneficial for investigating and efining the device's parameters . A comprehensive analysis is carried out using the SCAPS1D simulation in order to determine the photovoltaic device's maximum PCE . Variations were made to the temperature from 290 K to 350 K, the thickness of the absorbent layer from 0.1 to 1.1 µm, and the doping concentration level from 10^{12} cm^{-3} to 10^{18} cm^{-3} . After the simulation, the following values were obtained (PCE) = 19.72%, (FF) = 73.31 %, (Jsc) = 31.88 mA/cm^2 , and (Voc) = 0.68 V. The previously reported results were given for 10^{12} cm^{-3} , 0.7 µm, and 320 K

Key words: : SCAPS-1D,efficiency ,BaZrS3 , Chalcogenide perovskite, solar cells

Corresponding Email: wisbenaissa96@gmail.com

References

[1] Y.-Y. Sun et al., Chalcogenide perovskites for photovoltaics, Nano Lett. 15 (1) (2015) 581–585.

[2] S. Abdelaziz et al., Investigating the performance of formamidinium tin-based perovskite solar cell by SCAPS device simulation, Opt. Mater. 101 (2020),

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Finite element analysis of repair of composite laminates by bonding External patch

GHRIBI Saadiaa[a], M'hamdia Rachid[a]

[a] LMPA, departement of Mechanical Engineering, University of Technology, Sidi Bel Abbes , Algeria

Abstract:

Among the repair technologies, the external patch repair method is considered the easiest and fastest to work with. Still, there is potential for improvement in the performance of this mending technique. In this study, a unidirectional carbon/epoxy repair plate was used to repair a cracked plate in order to increase its life. The objective of this work is to compare the mechanical properties with an analytic study of cracking behavior before and after repairing the cracked plate. To achieve this objective the finite element method (Abaqus) is used. The obtained results clearly demonstrate that the service life and reliability of the repair are dependent on the mechanical properties of the structure that needs to be repaired.

Key words: External repair by bonding, Composite patch, Crack.

Corresponding Email: *saadia.ghribi@univ-sba.dz*

P-159

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Title: Monte Carlo study of the multilayer system and magnetic properties of the Site-disordered Blume Capel model.

Amel BENMANSOUR[a], Smaine BEKHECHI[a], Nabil Brahmi[a]

[a] *Department of Physics, Faculty of Sciences, Laboratory of* Theoretical Physics, *University of Tlemcen BP119, Algeria*

Abstract:

We used standard Monte Carlo simulations to investigate the magnetic properties of a spin-1 Ising multilayer system composed of two non-equivalent planes A and B, where B being site-diluted. Antiferromagnetic interlayer and ferromagnetic intralayer spin couplings have been considered. Our calculations indicated the occurrence of a compensation phenomenon where the magnetization vanishes before the critical temperature. The effects of various model parameters on the system magnetic properties have been examined in detail and presented in the form of phase diagrams. The results bore some resemblance with those reported in some previous works on systems with or without site-dilution. Depending on values of the spin concentration parameter P the model displayed first- and second-order phase boundaries with the existence of a tricritical point.

Key words: Blume Capel model , Multilayer spins system, Site dilution, Monte Carlo method, Compensation temperature, Tricritical point.

Corresponding Email:amel.benmansour93@gmail,com

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Composite pipelines susceptible to Hydrogen embrittlement : new proposal technics on the protection methods

Hayat Tati1, Mohammed Hadj Meliani 2 and Abdelnour Zaim3

Department of Mechanical Engineering, Mustapha Stambouli university of Mascara. Algeria

Department of Mechanical Engineering, University of Chlef

Abstract:

The study focuses on investigating the phenomenon of hydrogen embrittlement in both steel and composite pipelines, along with methods for protecting these pipelines from hydrogen-induced damage[1]. the proposed solution involves replacing traditional steel pipelines with composites composed of PHDE (Polyethylene high density) powder, silicium, and clay. Additionally, the study suggests a novel method of protecting these composite pipelines using a green inhibitor. Overall, the study aims to address the challenges associated with hydrogen embrittlement in pipelines by exploring alternative materials and protective measures. If successful, these findings could contribute to the development of more resilient and sustainable infrastructure for transporting fluids and gasses[2].

Key words: materials composite, hydrogen embrittlement, damage, triaxiality, crack, pipeline steel, notches, green inhibitor, pipeline composite.

Corresponding Email: email: hayet.tati@univ-mascara.dz

References

[1] Joshua Hoschke , Md Fahdul Wahab Chowdhury , Jeffrey Venezuela and Andrej Atrens, A review of hydrogen embrittlement in gas transmission pipeline steels, March 29, 2023.

[2] Jun Cao, Effect of hydrogen embrittlement on the safety assessment of low-strength hydrogen transmission pipeline, February 20242

P-161

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

A density functional theory study of the thermoelectric properties of $CuMg_2InS_4$

Hocine Hayat[a], Saadaoui Fatiha[a], Khelfaoui Friha[a], Ouafaa Sadouki[b], Amara Kadda[a].

[a] Department of physic, Laboratory of Physicochemical Studies, University of Saida-Dr. Moulay Tahar, Saida 20000, Algeria.
[b]Department of Matter Sciences, Faculty of Sciences and Technology, Tissemsilt University, Algeria.

Abstract:

This study presents a comprehensive investigation of the properties of the compound $CuMg_2InS_4$ chalcogenide using Density Functional Theory (DFT) simulation. The full potential linearized augmented plane wave plus local orbitals (FP-LAPW+lo) method with generalized gradient approximation (GGA) is employed to optimize its stannite (St), Kesterite (KS), Wurtzite Stannite (WS), and monoclinic (Pc) phases. The calculations show that $CuMg_2InS_4$ is a direct band gap semiconductor, with a band gap of 1.64 eV, in its structural ground phase, which is WS phase. The study further analyzes the structural, mechanical, electronic and thermoelectric properties of this phase. By utilizing the modified Becke-Johnson potential (TB-mBJ), $CuMg_2InS_4$ is a thermoelectric material with low thermal conductivity and high power factor. These results provide crucial insights into the characteristics of $CuMg_2InS_4$, which have significant practical applications in various fields such as energy conversion and electronic devices.

Keywords

FP-LAPW, DFT, stability, semiconductor, thermoelectric properties.

Corresponding Email:
hocine.hayat16@gmail.com

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Synthesis and characterization of a new chelating foaming phenolic resin for extraction of rare earths elements

Fatima BEKKAR[a,b,c], Radja MEGHERBI[b], Rachid MEGHABAR[c], Guilhem ARRACHART [a] and Stephane PELLET-ROSTAING[a]

[a] BEKKAK , ICSM, Univ Montpellier, CEA, CNRS, ENSCM, Marcoule, France

[b] MEGHERBI, Université des Sciences et de Technologies USTO-MB

[c] MEGHABAR, laboratoire de chimie des polymères, Université Oran 1, Oran, Algérie,

Abstract:

A few decades ago, polymer foams – materials that have since consisted of a gaseous phase dispersed in the form of cells in a solid polymer phase – have been increasingly used in industry. Their porous (alveolar) matrix gives them interesting mechanical properties combined with low density. This reduction in mass enables lower costs and energy savings in the case of transport or aerospace, and therefore a lower carbon footprint. Polymer foams are provided as versatile platforms that meet needs in various fields such as civil engineering, environment, health and energies. Among several types of polymeric foams, phenolic foams (PF) are characterized by a combination of properties that make them attractive - such as sound insulation, thermal insulation, sealing, energy absorption and protection against damage fire - which it is easy to orient towards a specific application. Thus, in order to provide an alternative to the industrial processes, which are harmful to the environment currently used for the extraction of rare earths[1,2] , namely liquid-liquid extraction, a difficult, expensive and above all polluting extraction technique. Polymeric foams based on phenolic foams prove to be solid supports which can be used as absorbents in solid-liquid extraction which have many advantages including the elimination of organic solvents, through their functionalization by a ligand of the diglycolamide type known for its selectivity towards heavy rare earths[3-5].

In this present study, we synthesized a new series of functionalized phenolic foam-based sorbents for the extraction of rare earth elements. Chelating phenolic foams were prepared using a suitable formulation of foaming agent, surfactant, curing agent and pre-polymer resulting from a polycondensation reaction under alkaline condition of a diglycolamide acid derivative with a mixture of phenol, catechol or resorcinol in the presence of formaldehyde as a cross-linking agent. Phenolic foams have been used, as a solid support in solid-liquid extraction, and evaluated for the extraction of three types of lanthanides (lanthanum La,

Europium Eu and ytterbium Yb) which represent the light, medium and ytterbium rare earths respectively heavy.

Key words: Phenolic Foam, Absorbent Materials, Diglycolamide, Rare Earth Elements, Liquid-Solid Extraction.

Corresponding Email: fatima.bekkar@univ-usto.dz, fbekkar@yahoo.fr

---

References

[1] eisman, D., Weber, R., Mckernan, J., & Northeim, C. **(2013)**. Rare Earth Elements: A Revieof Production, Processing, Recycling, and Associated Environmental IssueEnvironmental Protection Agency, Washington, DC.

[2] Blengini, G.A.; EL Latunussa, C.; Eynard, U.; Torres de Matos, C.; Wittmer, D.; Georgitzikis, KC. ; Carrara, S.; Mancini, L.; Unguru, M.; et al **(2020)**. Study on the Review of the List of Critical Raw Materials; European Commission: Brussels, Belgium.

[3] Binnemans, K., Jones, P. T., Blanpain, B., Van Gerven, T., Yang, Y., Walton, A., & Buchert, M**. (2013).** Recycling of rare earths: a critical review. *Journal of cleaner production*, *51*, 1- 22.

[4] Arrachart, G., Kenaan, A., Gracia, S., Turgis, R., Dubois, V., & Pellet-Rostaing, S. **(2015)** Design and Evaluation of Chelating Resins through EDTA-and DTPA-Modified Ligands. Separation Science and Technology, 50(12), 1882-1889.

[5] Arrambide, C., Arrachart, G., Berthalon, S., Wehbie, M., & Pellet-Rostaing, S. **(2019).** Extraction and recovery of rare earths by chelating phenolic copolymers bearing diglycolamic acid or diglycolamide moieties. *Reactive and Functional Polymers*, *142*, 14.

[1]

P-163

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Etude de l'effet de l'incorporation de nanocristaux et de nanofibres de chitine sur la structure et propriétés de l'hydroxypropyl méthylcellulose (HPMC)

Fatma Larbi*[a,b,c] , Ahmed Hamou[a] , Naceur Belgacem[b] et Julien Bras[b,c]

[a] LARBI , Département de chimie, Université Oran 1 Ahmed Ben Bella, El M'naouar, 31000 Oran, Algerie

[b] HAMOU , Univ. Grenoble Alpes, CNRS, LGP2, F-38000 Grenoble, France,
[c] JULIEN, IUF, F-75000 Paris, France.

Résumé

Les nanocristaux (NCchit) et nanofibres (NFchit) de chitine sont considérés comme des nanomatériaux prometteurs à fort potentiel d'innovation pour les domaines académiques et industriels. La recherche liée à leur production et à leur application est encore récente. D'autre part, de nombreux programmes de recherche sont concentrés ces dernières années sur le développement d'emballages de plus en plus biodégradables à base de polymères issus de ressources renouvelables. Parmi ces polymères, l'hydroxypropyl méthylcellulose (HPMC) est un dérivé cellulosique, de par sa nature hydrophile, sa structure chimique non toxique (Shetty et al., 2015) et son aptitude à la biodégradation, se distingue par des propriétés particulièrement intéressantes. Ce polymère qui a montré d'excellentes propriétés filmogènes (Villalobos et al., 2005) est devenu un matériau très attractif pour des applications dans le secteur de l'emballage dit « emballage comestible », pour cela ils doit avoir de bonnes propriétés mécaniques afin de conserver son intégrité lors de la manipulation du produit alimentaire sur lequel il est appliqué et aussi avoir de bonnes performances barrières à la vapeur d'eau et à l'oxygène.

Notre travail porte sur l'incorporation de NCCh et NFCh, produits par hydrolyse acide et par défibrillation mécanique respectivement, comme charges de renfort dans ce polymère afin de produire des films nanocomposites. Ces films ont fait l'objet d'une caractérisation en termes de propriétés morphologiques, structurales et thermiques. Un intérêt particulier a été porté, dans ce contexte, à l'influence du type et du taux de charge sur les propriétés mécaniques et barrières de ces nanocomposites

Les NFCh et les NCCh obtenus avaient des formes géométriques similaires sous forme de bâtonnets individualisés avec des tailles différentes. Les NFCh avaient un diamètre de 8,7 ± 3,2 nm et une longueur moyenne de 673,9 ± 263,3 nm, tandis que les NCCh avaient un diamètre de 9,7 ± 3.2 nm et une longueur moyenne de 243,5 ± 55,1 nm.

D’une manière générale et en termes de comparaison entre les performances des NCCh et des NFCh, les NCCh semblaient présenter un bon compromis entre les différentes propriétés étudiées, notamment les propriétés optiques et mécaniques ainsi que les propriétés barrières à la vapeur d’eau et à l’oxygène.

Mots clés : chitine, nanofibres, nanocristaux, composite, emballage, propretés barrières propriétés mécaniques.

Corresponding Email: larbi.fatma@univ-oran1.dz , fatmalarbi10@gmail.com

---

References

[1] Shetty, G.R., Rao, B.L., Asha, S., Wang, Y., Sangappa, Y., 2015. Preparation and characterization of silk fibroin/hydroxypropyl methyl cellulose (HPMC) blend films. Fibers Polym. 16, 1734–1741.

[2] Villalobos, R., Chanona, J., Hernández, P., Gutiérrez, G., Chiralt, A., 2005. Gloss and transparency of hydroxypropyl methylcellulose films containing surfactants as affected by their microstructure. Food Hydrocoll. 19, 53–61.

P-164

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Title: A first-principles investigation of the structural, mechanical, electrical, and optical characteristics of a novel quaternary SrFZnAs compoundMechanical, electrical, optical, and structural characteristics of a novel quaternary SrFZnAs compound: An understanding from the ground up

Presenting author's Kheira Hamaida [a,b], Zakia Louins[a] , Merime Harmal [c] , …

[a] Laboratory of Materials (LABMAT) National Polytechnic School (ENP) of Oran, BP 1523 El Mnaouar, Oran, 31000, Algeria
[b]Faculty of Sciences and Technology University Belhadj Bouchaib of Ain Temouchent, 46000, Algeria
[c] d Laboratory of Materials Study and Optical Instrumentations Djillali Liab`es University of Sidi Bel Abb`es, 22000, Algeria

Abstract:

In order to study the structural, mechanical, electrical, and optical characteristics of the quaternary compound SrFZnAs, this work uses the Full Potential Linearized Augmented Plane Wave approach inside Density Functional Theory as implemented in the WIEN2k code. Our computed values of the tetragonal SrFZnAs equilibrium structural parameters agree well with the experimental data. The ductile character, mechanical stability, and resistance to elastic deformations of SrFZnAs are further revealed by our analysis of the bulk modulus, shear modulus, Young's modulus, Poisson ratio, Lamé coefficients, Debye temperature, and sound velocity. According to the computed band structure, SrFZnAs is a semiconductor with a 1.64 eV direct band gap. Additionally, our analysis of optical characteristics highlights the potential of SrFZnAs for solar applications and includes the real and imaginary components of the dielectric function, refractive index, reflectivity, and absorption coefficient.

Key words: ..... FP-LAPW SrFZnAs compound (Mechanical Electronic and optical) properties.

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Structures électroniques et propriétés magnétiques des nitrures de métaux de transition

TAYEBI Nadjia[1] , BLAHA Lamia Farah[1] and KHATIR Radjaa[2]

[1]Laboratoire Physico-chimie des Matériaux Avancés (LPCMA), Université Djillali Liabès, Sidi Bel- Abbès 22000, Alegria.
[2]Laboratory of Electrical Engineering and Materials (LGEM), The Higher School of Electrical and Energetic
Engineering (ESGEE), Oran, Algeria.

Abstract:

Actuellement les progrès technologiques et industriels dans différents domaines dépendent fortement de l'avancement de la recherche dans le domaine des matériaux dont de nouvelles caractéristiques doivent être prises en compte. Notre investigation sur ces composés renseigne sur les différentes propriétés électroniques et magnétiques.

Notre travail est consacré à l'exploration des propriétés électroniques et magnétiques des nitrures qui contiennent un élément de la famille des métaux de transition.

A cet effet, nous avons choisi de travailler avec la méthode **FP-LMTO**: (Full Potential Linear Muffin-Tin Orbital) dans le cadre de la théorie de la fonctionnelle de la densité (DFT) [1] en utilisant deux types d'approximations, la LDA et La LSDA [2], pour étudier les propriétés électroniques et magnétiques des nitrures de métaux de transition **XN (X= Cr, V, Co, Mn).**

Les résultats montrent que les composés CrN, VN, CoN et MnN ont des moments importants dans la phase rocksalt, par contre dans la phase Zinc-Blende, ils ont des moments faibles. L'atome qui a le moment le plus élevé est le Mn. les moments magnétiques atomiques des matériaux de transition Cr, V, Co et Mn sont les plus dominants par rapport aux autres atomes. Il est évident que le moment magnétique total de nos composés est principalement dû aux métaux de transition.

Il est clair que les matériaux CrN, VN, CoN, et MnN, présentent un caractère métallique dans les deux phases rocksalt et zinc-blende suivants les spins majoritaires et minoritaires.

P-167

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

The 3rd edition of the international conference on matériels science and engineering and their impact on the environment

LES ENJEUX DU BETON DRAINANT PAR LA METHODE DE DREUX GORISSE

Chaabane Lynda Amel [a], Ouhib Rachid [a], Bouyakoub Amel Zahira [a], Harrache Djamila[a], Boudelel Bochera[b], Medelci Djezzar Khadidja[b]

[a]Laboratoire Physico Chimie Es Materiaux Avances, Sidi Bel Abbes, Algeria.
[b]Student in Materials, Department of Civil Engineering and Public Works Faculty of Technology, DjillaliLiabes University, B P 89 SidiBel Abbes, Algeria.

Abstract:

Le béton drainant (également appelé béton poreux, le béton perméable) est un type particulier formulé pour obtenir une forte porosité afin de permettre l'absorption et le drainage de l'eau ; utilisé en dallages, chaussées. Ce béton est généralement utilisé pour ses caractéristiques drainantes, d'ailleurs ces dernières décennies ont été marqué par une utilisation croissante du béton drainant dans le monde. Les applications les plus courantes sont : les aires de stationnements, les routes piétonnes et carrossables, les piscines, air de jeux, terrain de tennis. Néanmoins le béton drainant possède des caractéristiques mécaniques faibles comparées au béton ordinaire, ceci est dû à sa porosité effective relativement importante Dans cette étude, un intérêt particulier est porté sur le béton drainant appeler aussi béton perméable ou caverneux, à travers ce travail nous allons confectionner un béton drainant et l'étudier, pour ce faire, une caractérisation générale des matériaux utilisés a été faite, suivi de l'étude de la fabrication du béton étudié. Ensuite des essais mécaniques ont été réalisés à différents âge du béton.

Le béton perméable (également appelé béton poreux, béton perméable) est un type particulier formulé pour atteindre une porosité élevée afin de permettre l'absorption et le drainage de l'eau ; utilisé dans le pavage, les trottoirs. Ce béton est généralement utilisé pour ses

caractéristiques drainantes, et les dernières décennies ont été marquées par une utilisation croissante des bétons drainants à travers le monde. Les applications les plus courantes sont : les aires de stationnement, les routes piétonnes et carrossables, les piscines, les terrains de jeux, les courts de tennis. Cependant, le béton perméable présente des caractéristiques mécaniques faibles par rapport au béton ordinaire, cela est dû à sa porosité effective relativement élevée. Dans cette étude un intérêt particulier est porté sur les bétons perméables, encore appelés bétons perméables ou caverneux, à travers ce travail nous allons réaliser un béton perméable et l'étudier, pour ce faire, une caractérisation générale des matériaux utilisés a été faite, suivie de l'étude de la fabrication du béton étudié. Ensuite des essais mécaniques ont été réalisés à différents âges du béton.

Key words: béton drainant- effet du sable- résistances mécaniques**.**

Corresponding Email: chaabane25@hotmail.com

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

The 3rd edition of the international conference on matériels science and engineering and their impact on the environment

Treatment of Textile Effluents by Combined Methods

Bouyakoub Amel Zahira [a] , Ouhib Rachid [a], Chaabane Lynda Amel[a], Harrache Djamila[a], Belhadj Hafida[a]

[a]Laboratoire Physico Chimie Es Materiaux Avances, Sidi Bel Abbes, Algeria

Abstract :

The treatment of effluents by coagulation-electroflotation was studied. The study aims to optimize the treatment conditions which maximize the efficiency of the purification. pH and current density are the most important factors in dye removal. The efficiency of purification consisting of the removal of suspended matter exceeded 90%. A physicochemical characterization of the effluent was carried out before and after treatment.

Keywords: dyes,Pollution, coagulation-electroflotation, current density, Treatment

Corresponding Email: zbouyakoub@yahoo.fr

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

The 3rd edition of the international conference on matériels science and engineering and their impact on the environment

Removal Of Azo-Dye From Synthetic Wastewater By Coagulation

Rachid Ouhib[a], Chaabane Lynda Amel[a], Amel Zahira Bouyakoub[a] , Harrache Djamila[a], Belhadj Hafida[a]

[a]Laboratoire Physico Chimie Es Materiaux Avances, Sidi Bel Abbes, Algeria

Abstract

Highly soluble azo dyes are commonly used due to their advantages such as good dyeing processing conditions and good fixation on all types of fibers. But the resulting effluents are characterized by low biodegradability, high alkalinity, a large quantity of suspended solids (MES), and chemical oxygen demand (COD). Documentation of these discharges must be processed beforehand in order to comply with environmental protection laws for receiving waters.

Keywords: azo dyes, Pollution, COD, MES, Treatment

Corresponding Email : r_ouhib@yahoo.fr

P-170

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

The 3rd edition of the international conference on matériels science and engineering and their impact on the environment

Etude des propriétés structurales, électroniques et thermodynamiques d'un alliage quaternaires Cu_2CdSnS_4 par la méthode du potentiel total-linéaire des orbitales muffin-tin (FP-LMTO)

Belkhouane Samira[a], Rachid Ouhib[a], Chaabane Lynda Amel[a], Amel Zahira Bouyakoub[a] , Yarub Al-Douri[b]

[a]laboratoire Physico Chimie Es Materiaux Avances, Sidi Bel Abbes, Algeria

[b] American University of Iraq, Sulaimani.

Abstract :

La conception et la fabrication de ces nouveaux matériaux, aux propriétés souvent étonnantes constitue un domaine très actif de la recherche et de la technologie moderne. Les alliages quaternaires Cu_2CdSnS_4 utiles pour les applications photovoltaïques, ont été synthétisés avec succès sur des substrats en silicium de type p en utilisant la technique de revêtement en spin à différentes températures de recuit jusqu'à 500°C. Les propriétés optiques ont été étudiées par des spectrofluoromètres UV-vis et photoluminescence (PL). Ces nanostructures ont un écart de bande d'énergie direct de 1,29 à 1,31 eV. Nous nous intéressons d'abord aux alliages quaternaires, car ils ont beaucoup

Keywords: alliages quaternaires, propriétés structurales, FP-LMTO, photovoltaïques.
Corresponding Email : belkhouanes@yahoo.fr

P-171

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Synthesis and characterisation of triple-reponsive copolymer hydrogels based on 2-(dimethylamino)ethyl methacrylate and acrylic acid : an intelligent materials chemically cross-linked developed for treatment and dyes removal

Badaoui Asmaa[a], Chaibi Wahiba[b] , Guemra Kaddour[c]

[a] PhD candidate, Laboratory of Physical and Macromolecular Organic Chemistry (LCOPM), "Djillali Liabes" University of Sidi Bel Abbes, BP 89, Faculty of Exact Sciences, Algeria.

[b] Research Master A, Scientific Research Center for Physicochemical Analysis Techniques (CRAPC), Bousmail, RP 42415, Tipaza, Algeria.

[c] Professor- Laboratory of Physical and Macromolecular Organic Chemistry (LCOPM), "Djillali Liabes" University of Sidi Bel-Abbes, BP 89, Faculty of Exact Sciences, Algeria.

Abstract:

Industrial activities have led to environmental contamination, particularly by heavy metals and industrial dyes, which are the main pollutants of water resources in many parts of the world. These contaminants pose not only an aesthetic but also a health problem, as the molecules contain carcinogenic groups that alter the genetic code, leading to mutations and the risk of cancer. The remarkable adsorption characteristics and porous morphology of hydrogel polymers make them widely used in the environmental industry as depollutants, capable of adsorbing large quantities of industrial fluids such as dyes without disintegrating.

The objective of this study is to develop smart hydrogel polymers that are sensitive to different temperature, pH, and salinity stimuli. This will be achieved by modifying the molar proportions of 2-[N,N-Dimethylamino]ethyl methacrylate (DMAEMA) and acrylic acid (AA) (60/40 to 40/60). The resulting hydrogels were synthesized by a radical copolymerization

process using potassium persulfate (KPS) and N,N-methylene bis-acrylamide (MBA) as initiator and cross-linking agent, respectively. The hydrogels were characterized by Fourier transform infrared spectroscopy (FTIR) and scanning electron microscopy (SEM) to determine their remarkable structural and morphological properties.

A study was conducted to examine the swelling properties of the hydrogels under varying temperature, pH, and salt conditions. The swelling rate was calculated for each case. Additionally, a study was performed to assess the retention of Bemacide red, a water-soluble dye commonly utilized in textiles to treat and sanitize wastewater by reducing its toxicity, at different concentrations.

Key words:

Smart hydrogels; free-radical copolymerization; 2-[N,N-Dimethylamino]ethyl methacrylate; acrylic acid; swelling behavior ; Bemacid red retention

Corresponding Email: asmaabadaoui022@gmail.com

P-172

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Free vibration analysis of porous multi-directional FG sandwich plates

Lazreg Hadji[1,2*], Nafissa Zouatnia[1], Latifa Ould Larbi[3], Royal Madan[4]

[1] Department of Civil Engineering, University of Tiaret, BP 78 Zaaroura, Tiaret, 14000, Algeria.
[2] Laboratory of Geomatics and Sustainable Development, University of Tiaret, 14000, Algeria.
[3] Laboratory of Structures, Geotechnics and Risks, Department of Civil Engineering, Hassiba Benbouali University of Chlef, Algeria.
[4] Department of Mechanical Engineering, Graphic Era (Deemed to be University) Dehradun- 248002, India.

Corresponding author : lazreg.hadji@univ-tiaret.dz

Abstract

Free vibration analysis of multi-directional porous functionally graded (FG) sandwich plate has been performed for two cases namely: FG skin with homogeneous core and FG core with homogeneous skin. Hamilton's principle was employed and the solution was obtained using Navier's technique. This theory imposes traction-free boundary conditions on the surfaces and does not require shear correction factors. The results obtained are validated with those available in the literature. The composition of metal-ceramic-based functionally graded material (FGM) changes in longitudinal and transverse directions according to the power law. Imperfections in the functionally graded material introduced during the fabrication process were modeled with different porosity laws such as evenly, unevenly distributed, and logarithmic uneven distributions. The effect of porosity laws and geometry parameters on the natural frequency was investigated. On comparing the natural frequency of two cases for perfect and imperfect sandwich plates a reverse trend in natural frequency result was seen. The finding shows a multi-directional functionally graded structures perform better compared to uni-directional gradation. Hence, critical grading parameters and imperfection types have been identified which will guide experimentalists and researchers in selecting fabrication routes for improving the performance of such structures.

Keywords: FGM sandwich plate; free vibration; multi-directional FGM; Navier's solution; Porosity effects.

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Numerical Simulation of heat transfer of hybrid nanofluid In PV/T solar panel

Souad Benkherbache[a],

[a]Department of Mechanical Engineering, Faculty of Technology, University of Mohamed Boudiaf-M'sila, Algeria

Abstract:

This work represents a 3D numerical study of heat transfer of a hybrid nanofluid in the tube of a hybrid photovoltaic solar panel PV/T .The Fluent 6.3.26 software packages is used to carry out the numerical simulations. The hybrid nanofluids composed of TiO_2-Cu/water and TiO_2-Ag/water suspension. The properties of these hybrid nanofluids can be influenced by the type, size, and concentration of nanoparticles. As independent control factors, the nanoparticles concentration ratio in the hybrid nanofluid were employed. The thermal efficiency and the temperature of the PV/T components were employed as dependent parameters. According to the simulation data, the thermal efficiency and the temperature of the PV/T system increased by increasing the volume concentration of the nanoparticles. The hybrid nanofluid TiO_2-Ag/water gives the best efficiency than TiO_2-Cu/water

Key words: Hybrid nanofluid, pv/T solar panel, heat transfer, numerical simulation

Corresponding Email:

References

[1] souad.benkherbache@univ-msila.dz

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Free vibration analysis of FG sandwich beams with porosity

Guermit Mohamed Bilal CHAMI[a], Lazreg Hadji[b], Abdelkader SAFA[c], Latifa Ould Larbi[d],

[a] Department of Civil Engineering, Mouloud Mammeri University, Tizi Ouzou, Algeria.
[b] Department of Civil Engineering, University of Tiaret, Algeria.
[c] Department of Civil Engineering, University of Relizane, Algeria.
[d] Laboratory of Structures, Geotechnics and Risks, Department of Civil Engineering, Hassiba Benbouali University of Chlef, Algeria.

Abstract:

In this paper, a simple n-order refined theory is developed for free vibration of a simply supported sandwich beam with functionally graded porous layers. The present theory is variationally consistent, uses the n-order polynomial term to represent the displacement field, and does not require a shear correction factor. The variation of shear stress is parabolic across the thickness and the condition at the top and bottom surface are shear stress-free. Equations of motion are derived from Hamilton's principle. In the solution of the governing equations, the Navier procedure is implemented. For porosity effect, four different porosity distributions namely O, X, V, and homogeneous distribution types are modelled; power-law variation of functionally graded face sheets is considered. Results show the effects of varying gradients, thickness to length ratios, and porosity types on free vibration of functionally graded sandwich beams for simply supported boundary conditions. The results of the present method were validated with existing literature for both hard (ceramic) core material and soft (metal) core material, and good agreement with the benchmarks is seen. The effect of hard-core and soft-core material on natural frequency is found to be contrasting in nature.

Key words: Porosity, Free vibration, FGM, Navier solution, Functionally graded sandwich beams.

Corresponding Email: guermit.chami@yahoo.com

P-175

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Title: Effect of swap defect on the electronic and magnetic properties of quaternary heuslers alloys

Latreche Laid[a,b], Dr .Hamza Abbassa[a,b]

[a]Authors' Physics departement, Faculty of Exact Sciences and Computer Science, University of Mostaganem, Algeria
[b]Authors' ECP3M Laboratory, University of Mostaganem, Algeria

Abstract:

Quaternary Heusler alloys are promising for spintronics data storage, energy conversion and optoelectronics, but swap defects can significantly alter their properties. These defects, which involve atoms exchanging places, can affect electronic and magnetic behaviors, influencing half-metallicity and spin polarization. Understanding and controlling these defects is crucial for optimizing the alloys' performance in technological applications.

Key words: Quaternary Heusler alloys, Swap defects, Electronic properties, Spintronics

Corresponding Email: latreche.laid@gmail.com

References

[1] Defects in solids. (2008). J. Wiley and Sons.

[2] Felser, C., Fecher, G. H., & Balke, B. (2007). Spintronics: A challenge for materials science and solid-state chemistry. *Angewandte Chemie International Edition*, *46*(5), 668–699. https://doi.org/10.1002/anie.200601815

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Title: Analyse Dynamique des nano-structures en FGM

Bendaida Mohamed[a,*], Boutaleb Sabrina[b], Tounsi Abdeldjebbar[b], Bourada Fouad[b] , ***Houari Heireche*** [a]

[a] Laboratory of Modelisation and simulation multi echelle Univrsity of Sidi Bel Abbes, Sidi Bel Abbes, Algeria
[b] Laboratoire des Matériaux et Hydrologie Université Djillali Liabes de Sidi Bel Abbes, Algeria

Abstract:

Dans ce travail, l'impact de la temperature sur la vibration libre des Nano-structures fonctionnellement graduées (FG) sont analysé en utilisant une nouvelle théorie TBT nonlocale à deux inconnues pour la première fois.. Le principal avantage du modèle proposé est que, en plus de considérer à la fois la déformation de cisaillement et les effets non locaux, la cinématique est modélisée par seulement "deux inconnues" comme le modèle de "la théorie classique des poutres" (CBT) et qui est encore meilleur que le modèle de "la théorie des poutres de Timoshenko" (TBT). Les caractéristiques du matériau dépendant de la température du "Nanopoutre FG" sont considérées comme variables de manière continue dans l'épaisseur selon "la forme de la loi de puissance". Les "équations de mouvement" non locales sont obtenues en utilisant le "principe de Hamilton" et sont résolues en appliquant la "solution analytique". Les impacts des environnements thermiques, de l'indice de matériau et des paramètres non locaux sur les propriétés dynamiques des Nanopoutre FG sont discutés.

Key words: . vibration libre, Nanopoutre FG, loi de puissance, principe de Hamilton

Corresponding Email:
bendida65@gmail.com

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Study of the spin collapse in orthoferrite using LDA+U

AMERI Ibhraim[a], BLAHA Lamia Farah[a], KHATIR Radja[b]

[a]University Djillali Liabbes Sidi Bel Abbes . Physico-Chemiistry Laboratory of Advanced Materials
[b] Laboratory of Electrical Engineering and Materials (LGEM), Oran, 31000, Algeria

Abstract:

Rare-earth (R) orthoferrites RFeO3 exhibit large volume transitions associated with a spin collapse. We present here *ab initio* calculations on RFeO3(R= Pr, Nd). We show that taking into account the strong correlation among the Fe-3d electrons is necessary. Indeed, with the LDA+U method in the projector augmented wave, we are able to describe the isostructural phase transition at 50 GPa, as well as a volume discontinuity of 6.0% at the transition and the considerable reduction in the magnetic moment on the Fe ions [1]. We further investigate the effect of the variation in U and J and find a linear dependence of the transition pressure on these parameters. We give an interpretation for the nonintuitive effect of J [2]. This emphasizes the need for a correct determination of these parameters especially when the LDA+U is applied to systems (e.g., in geophysical investigations) where the transition pressure is a priori unknown

Key words: LDA+U , orthoferrites , isostructural.

Corresponding Email: ameriibrahim22@gmail.com

References

[1] K. Aizu, Phys. Rev. B 2 (1970) 754.

[2] S.-W. Cheong, M. Mostovoy, Nat. Mater. 6 (2007) 13.

P-178

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Identifiquation d'une plante endimique de la region

Sud ouest algerien.

Belkralladi.Halima [a] , Djamaa.Z [c] , bouyakoub.Z [b] , Oughilas.A [a] ,Kaid Omar.Z [a]

[a]Belkralladi.Halima a faculté science exacte département de Chimie, Sidi belabbes, Algerie.

[b]Laboratoire PHYSICO CHIMIE ES MATERIAUX AVANCES (LPCMA), SIDI BEL ABBES, ALGERIA

Abstract:

L'utilisation des plantes en phytothérapie est très ancienne et connaît actuellement une région d'intérêt auprès du public, selon l'Organisation Mondiale de la Santé (OMS) environ 65-80% de la population mondiale à recours au médicine traditionnelle pour satisfaire ses besoins en soins de santé primaire, en raison de la pauvreté et du manque d'accès à la médecine moderne. Le genre zygophyllum est le plus répandu de la famille des Zygophyllaceae. Ce sont des plantes très adaptées au milieu désertique par leur système de racines horizontales qui parcourent de longues distances et absorbent

la moindre goutte d'eau. Quelques études sur cette plantes montrent que Zygophyllum album pourrait exercer leurs activités antidiabétiques grâce à leurs propriétés antioxydantes, son extrait montre une diminution significative de l'activité du glucose sanguin, de la peroxydation des lipides dans le foie et le pancréas et une augmentation significative des antioxydants enzymatiques et non enzymatiques. Les principaux constituants décrits à partir de Zygophyllum album sont glycosides, stérol, des tanins, protéines / acides aminés, des saponines, triterpènes et flavonoïdes. L étude s'est portée sur le Zygophyllum album en les caractérisant par une identification de certains composés phénoliques par chromatographie (GSM) et une évaluation des activités antioxydant.

Key words: ethnobotanique, zygophyllum, Sahara, antioxydant, chromatogramme, G.S.M,

poly- phénols.

Corresponding Email:

_____

halima.belkralladi@univ-sba.dz

belkralladihalima@yahoo.fr

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Influence of Polymer Types and Concentrations on Losartan Controlled Release Microparticles

Meryem Mouffok[a,b], Awatif Amaria Moulay[a], Ilham Abdelmalek[a], Abderrezzak Mesli[a], Kaddour Guemra[a]

[a]Laboratory of Physical and Macromolecular Organic Chemistry, Djillali Liabes University of Sidi Bel-Abbes, Algeria
[b]Electronics Department, Electrical Engineering Faculty, Djillali Liabes University of Sidi Bel-Abbes, Algeria

Abstract:

Losartan-loaded Microsparticles were prepared by emulsion-solvent evaporation method using ethyl cellulose (EC) as polymer carrier. This technique includes several steps that have been developed in order to attain a better control over the whole process and to achieve an important delayed effect.The effects of process conditions such as : polymer types and concentrations, volume ratio of oil to water emulsion on the Microparticles properties were studied in order to investigate their effect on the encapsulation efficiency and drug release kinetics. The obtained Microsparticles were characterized by SEM, DRX and FTIR and the size dispersion was also determined. The release of Losartan was performed in simulated gastric medium (pH=1.2) at 37±0.5 °C using UV–Vis analysis. Data obtained from in-vitro drug release from microparticles were fitted to various kinetic models. Drug release kinetics corresponds better to Higuchi model.

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

THE WINKLER FOUNDATION STIFFNESS EFFECT ON THE VIBRATION CHARACTERISTICS OF FGM NANO-BEAM USING THE FINITE ELEMENT METHOD

Ghali Drici[a], Ismail Mechab[a], Noureddine Elmeiche [c]

[a] Department of Mechanical Engineering, Laboratory Mechanics Physics of Materials (LMPM), University of Sidi Bel Abbes, Sidi Bel Abbes, Algeria.
[b] Civil and Environmental Engineering Laboratory (LGCE), Department of Civil Engineering and publics' works, Faculty of Technology, Djilali Liabes University, Sidi Bel Abbes, Algeria .

Abstract:

This work analyses the winkler foundation stiffness on vibration characteristics of Functionally Graded Materials (FGM) viscoelastic nano-beams resting on Winkler-type viscoelastic foundations, based on Eringen's non-local deformation gradient theory of elasticity using the finite element method. The viscoelastic foundation consists of a Winkler layer and a viscous layer based on the infinite Kelvin-Voigt model. A power law model is used to describe the continuous variation of the material properties of the FGM nano-beams. In order to validate the model presented, the results are compared with those of the elastic nano-beam found in the literature. The effects of winkler stiffness , foundation damping coefficient, on the frequency response of viscoelastic nano-beam are studied.

Key words: winkler stiffness , FGM , non-local, nano-beam.

Corresponding Email: ghalidrici22@gmail.com

References

[1] N. C. A.E. Alshorbagy, M.A. Eltaher, F.F. Mahmoud, " Free vibration characteristics of a functionally graded beam by finite element method ", Applied Mathematical Modelling, 35.412–425,2011 .

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Deformation and Electronic Properties of Amorphous Tubes under the Influence of Electric Fields

F. BAIRA[a,*], Y. Benkrima [b], S. ZIDANI[c]

[a] Université de Batna2.05078 Batna, Faculté de technologie, Algerie, Département de science et technologie
[b] Department of Exact Sciences, ENS Ouargla, Algeria.
[c]Université Batna 1 el hadj lakhdar. 05000 Batna Algérie, Université, Département technologie alimentaire, laboratoire des sciences des aliments LSA

Abstract:

The structural and electronic properties of pure ZnO nanotubes were investigated in zigzag (5,0) (7,0) (9,0) (5,5) (7,7) (9,9) and armchair (5,5) (7,7) (9,9) states and comparatively using density function theory (DFT) and generalized gradient approximation (GGA). The results show that the strain energy of ZnO nanotubes increases with increasing diameter and that their energy bands are semiconducting energy bands, which compare favorably with those recorded in the bulk zinc oxide state using this theory, and that the decrease in energy band values is related to the increase in diameter Applying an electric field to ZnO nanotubes deforms them, the deformation increases with the increase in the value of the electric field, the rate of strain increases with the increase in the diameter of the ZnO nanotubes as well, and increasing the electric field applied to them decreases the value of their energy gap.

Key words: Ab-initio study, ZnO nanotubes, electric field, strain energy, band structure.

Corresponding Email: f.baira@univ-batna2.dz

References

[1] F. Baira, S. Zidani, J. Tob Regul. Sci. 1,9. 3654-3662 (2023).

[2] Y. Achour, Y. Benkrima, I. Lefkaier, D. Belfennache, J. Nano- Electron. Phys. 15, 01018 (2023).

P-182

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

REUSE WASTEWATER

Awatif Amaria Moulay[a], R. OUHIB[b], K.DJAHAF[b], Meryem Mouffok[a,c], A. Z. BOUYAKOUB[b]

Laboratory of Physical Chemistry of Advanced Materials (LPCMA) Sidi-Bel-Abbes, Algeria

[a]Laboratory of Physical and Macromolecular Organic Chemistry, Djillali Liabes University of Sidi Bel-Abbes, Algeria
[b] Laboratory of Physical Chemistry of Advanced Materials (LPCMA) Sidi-Bel-Abbes, Algeria
[c]Electronics Department, Electrical Engineering Faculty, Djillali Liabes University of Sidi Bel-Abbes, Algeria

Abstract:

Population growth, increased economic activities and expansion of irrigated agricultural areas are the main reasons for the increase in water demand. Therefore, the recovery and reuse of wastewater has become a necessity, even a priority due to the role it plays in reducing freshwater consumption and wastewater production, but a very limited due to legal obligations, costs and hygiene concerns. Recycled water is a reliable water source that must be taken into account when developing a sustainable water policy.

Key words: Wastewater, Reuse, Recycledwater.

Corresponding Email:
awatif_amaria@yahoo.fr

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Prediction of materials with high thermoelectric efficiency at high pressure

Maoudj Hanane, H. CHORFI , A. BOULTIF

Abstract

The ultimate objective of this project is the proposal of new materials with high thermoelectric performance. The success in its achievement is associated with the fulfillment of two other intermediate objectives. The first is of a methodological nature and consists on the combination of prediction models of crystalline structures (XtalOpt, USPEX, …) with strategies for chemical-quantum calculation of electronic, thermodynamic and transport properties (VASP+newGIBBS). The second is of an applied nature. It seeks to obtain property-structure correlations from the computational exploration of regions of increasing pressures in the phase diagram of families of compounds with high value of the figure of merit (ZT) (AgCl, PbTe, SnSe, CoSb3) and allowing stoichiometric variations. The joint action of the computational tools and techniques along with their application is a unique opportunity to provide a better understanding of the parameters involved in ZT and advance in the rational design of materials that efficiently convert heat into electrical energy.

P-184

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Syntheses and Characterization a magnetic composite modified by different Ctab concentrations for the removal of Sm(III) from aqueous solutions

C.Hanagria[1], B. Haddou[1*], A. Debbeb[2], I.Ameri[3]

[1]Laboratory of Physical Chemistry of Materials: Catalysis and Environment, Faculty of chemistry University of Science and Technology of Oran, BP 1505, M'Nouar, Oran, Algeria

[2]·Laboratory of engineering and environmental processes, faculty of chemistry,

University of Science and Technology of Oran, BP 1505, M'Nouar, Oran, Algeria

[3]Laboratory of Physical Chemistry of Advanced Materials (LPCMA)

University of Djillali Liabes, BP 89, 22000, Sidi-Bel-Abbes, Algeria

Abstract:

In this study, we synthesized a magnetic composite based on illite and functionalized Fe_2O_3 with sodium folate (C19H18N7NaO6) for the removal of Sm(III), Various characterization techniques were used including X-Ray diffraction, vibrating sample magnetometry (VSM), balayage electron microscopy (MEB) , fourier-transform infrared spectroscopy (FTIR) , thermogravimetric analysis (TGA), and zeta-sizer devices to analyze the magnetic composite . The optimization study of the adsorption operating conditions revealed that the optimum pH for the adsorption of all metals is 6, Isotherm calculations indicated that the langumir and sips model provide the best fit R^2 superieur à 0.9, suggesting the occurrence of two types of adsorption : physic-sorption and chimi-sorption, the adsorption capacities of Sm(III) are found to 40 mg/g. The pseudo 2 nd

order model was determined to be the best fit for the kinetics of adsorption . The negative values of ΔG° obtained at all three temperatures indicate the spontaneity and feasibility of the adsorption processus on the magnetic composite. However, the degree of spontaneity decreases with increasing temperature. Nitric acid (0.5 M) was identified as the most effective éluant, the reusability of the mafnetic composite was demonstrated with all three metals after 4 cycles. Lastly, the magnetic composite proved to be effective in removing toxic metals from wastewater.

Key words: composite , metals , adsorption, illite, maghmite, adsorption,

Corresponding Email: hanagria.cherifachahrazed@gmail.com

References

[1] M. Shafiee, R. Foroutan, K. Fouladi, M. Ahmadlouydarab, B. Ramavandi, S. Sahebi, Application of oak powder/Fe3O4 magnetic composite in toxic metals removal from aqueous solutions, Adv. Powder Technol. 30 (3) (2019) 544–554.

[2] Z. Esvandi, R. Foroutan, M. Mirjalili, G.A. Sorial, B. Ramavandi, Physicochemical behavior of Penaeuse semisulcatuse chitin for Pb and Cd removal from aqueous environment, J. Polym. Environ. 27 (2) (2019) 263–274.

[3] C. Zhao, R. Ge, Y. Zhen, Y. Wang, Z. Li, Y. Shi, X. Chen, A hybrid process of coprecipitation-induced crystallization-capacitive deionization-ion exchange process for heavy metals removal from hypersaline ternary precursor wastewater, Chem. Eng. J. 378 (2019), 122-136.

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Experimental and numerical study of ZnO nanoparticles

CHEKROUN Mohamed Zoheir[a]

[a] University Djillali Liabbes Sidi Bel Abbes . Physico-Chemiistry Laboratory of Advanced Materials

Abstract:

In the realm of photonic devices, light-matter interaction has recently been a hot topic of study. In semiconductors, absorption management is critical for device performance, especially in plasmonic waveguides. Nanoparticles made of zinc oxide (ZnO) demonstrate confinement effects in the ultraviolet and visible ranges, making it a well-known material for numerous photonic applications. Confined modes are ideal for applications needing high-efficiency coupling from single-photon emitters, such as ultra-sensitive optical sensor systems. In this paper, we have performed an experimental and numerical study of ZnO nanoparticles deposited on a glass substrate by the spray pyrolysis technique. The structural properties of our samples have been determined by X-ray diffraction study, which revealed satisfactory crystallization in the wurtzite phase with a preferred peak at (200) orientation. Experimental measurements and theoretical modeling are divided into two components in the optical study. In the region of 250–2500 nm, the experimental measurements are made with a (JASCO type V-570 double-beam spectrophotometer), we have obtained the results of transmittance reflectance and absorption as a function of wavelength. Lastly, we have injected the refractive indices n and k of ZnO into the calculation code derived from the experimental results. The optical behavior of ZnO nanoparticles deposited on glass has been studied numerically with differential methods in both optical far-field and near-field. The numerical calculation results were carried out with a spectral study in the range of 250–800 nm as a

function of the incidence angle varying from 0 to 80°. We notice the presence of two very high absorption peaks at wavelengths of 280 nm and 366 nm, respectively

Corresponding Email: Chekrounmohamedzoheir@yahoo.com

ICMSE'2024

The 3rd Edition of the international conference on materials science and engineering and their impact on the environment

Wear behavior of copper alloys thermal spray coatings

Toufik MANA [a,*],

[a] Laboratory of Research in Mechanical Engineering and Materials, Military Academy of Cherchell Defunct President Houari Boumediene, Algeria.

Abstract:
In June 2008, ATRA Company in Béjaïa received its first shipment of Aluminum Bronze, a commercial material, in the form of a 3.5mm diameter wire. This wire was intended for refurbishing mechanical parts made of copper alloys. Through microstructural characterization using X-ray diffraction and EDX microanalysis with SEM, the phases developed by this material after thermal spraying using the wire flame process were identified. Surprisingly, the presence of the Cu_3Al compound was detected, which is normally stable above 586°C according to the Cu-Al equilibrium diagram. This finding was unexpected. The adhesion of this coating to the CuSn8 bronze biphasic substrate was found to be low. However, preheating the substrate to 80°C before thermal spraying significantly improved adhesion energy, increasing it nearly twentyfold. Mechanical tests revealed that the presence of Al and Zn bonding sublayers had a negative impact on the coating's adhesion to the CuSn8 bronze biphasic substrate. The friction coefficient of the coating stabilized at an average value of 0.42 under a load of 15N, while mass loss stabilized after 1 hour and 30 minutes under the same load.

Key words: Thermal spraying, coating, aluminium bronze, friction, wear.
***Corresponding Email** : toufik_mana@yahoo.com

References

[1] M. A. Bradai, M. Braccini, A. Ati, N. Bounar, A. Benabbas, "Microstructure and adhesion of 100Cr6 steel coatings thermally sprayed on a 35CrMo4 steel substrate", Surf. Coat.Techno., 202, PP. 4538-4541, 2008.

[2] T.MANA Multicomponent Al-Bronze coatings thermally sprayed onto tin bronze substrate: Microstructural, mechanical and corrosion characterization in a 3.5% NaCl solution Surface Review and Letters 27(04), 2019.

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Study of the electronic and magnetic properties of the double perovskite Ca2CoMoO6

Djefal Abdelkader , S.Amari , B. Bouhafs

Abstract

A systematic investigation on magnetism and spin-resolved electronic properties in double perovskite Ca2CoMoO6 compound was performed by using the full potential augmented plane wave plus local orbitals (APW+lo) method within the generalized gradient approximation (GGAPBE) and GGA-PBE+U scheme. The stability of monoclinic phase (P21/n #14) relative to the tetragonal (I4/m#87) and cubic (Fm_3 m #225) phase is evaluated. We investigate the effect of Hubbard parameter U on the ground-state structural and electronic properties of Ca2CoMoO6 compound. We found that the ferromagnetic ground state is the most stable magnetic configuration. The calculated spin-polarized band structures and densities of states indicate that the Ca2CoMoO6 compound is half-metallic (HM) and half-semiconductor (HSC) ferromagnetic (FM) semiconductor with a total magnetic moment of 6.0 using GGA-PBE and GGA PBE+U, respectively. The Hubbard U parameter provides better description of the electronic structure. Using the Vampire code, an estimation of exchange couplings and magnetic Curie temperature is calculated. Further, our results regarding the magnetic properties of this compound reveal their ferromagnetic nature. The GGA-PBE+U approach provides better band gap results as compared to GGA-PBE approximation. These results imply that Ca2CoMoO6 could be a promising magnetic semiconductor for application in spintronic devices..

P-188

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Title: A Theoretical Study Of A Dynamical Stability of A Novel Double Spinel Zinc Ferrite.

A. Hachilif[a], F. Khelfaoui[b], A. Bouhemadou[c], A. R. Benrekia[d], T. Djeldjeli [e].

[a] Computational Materials Physics Laboratory (CMPL), Faculty of Exact Sciences, Djillali Liabès University of Sidi Bel Abbès, Sidi Bel Abbès 22000, Algeria.
[b] Laboratory of Physicochemical Studies, Dr. Moulay Tahar University of Saida, Saida 20000, Algeria.
[c] Laboratory for Developing New Materials and their Characterizations, Department of Physics, Faculty of Sciences, Ferhat Abbas University – Setif 1, Setif 19000, Algeria.
[d]Yahia Fares university of Médéa, Médéa 26000, Algeria.
[e] Laboratory of Materials and Reactive Systems, University of Sidi-bel-Abbès, Sidi Bel Abbès 22000, Algeria.

Abstract:

Double spinel materials, ABB'O4, represent an emerging class of oxides with significant technological potential [1]. First-principles calculations were utilized to investigate the fundamental properties of the double spinel ZnFeSnO4. Employing the pseudo-potential plane wave (PP-PW) method, we analyzed the elasticity and dynamic stability of ZnFeSnO4[2]. The findings indicate favorable thermodynamic stability, mechanical robustness, and dynamic stability for ZnFeSnO4. Given the lack of previous investigations for direct comparison, future experimental studies are encouraged to confirm and further develop these results.

Key words: Double Spinel Oxides, Stability, thermodynamic stability.

Corresponding Email:
___hachilifasma@gmail.com_____

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

First principles study of the double perovskite compound Ba_2RhWO_6 for optoelectronic applications

M.Harmel[a], K.Hamaida[b]

[a]University of Science and Technology Mohamed Boudiaf of oran, Materials Technology Department, Oran 31000, Algeria.
[b] Ain Temouchent University Belhadj Bouchaib, 46000, Algeria.

Abstract:

A theoretical predictions on structural, electronic, magnetic and optical properties of Ba_2RhWO_6 double perovskite oxide has been effectively calculated using the full-potential linearized augmented plane wave method (FP-LAPW) based on the density functional theory (DFT). The exchange correlation potential is treated by the generalized gradient approximation (GGA) and GGA+U where U is on-site Coulomb interaction correction. Our structural study shows that the compounds have cubic symmetry. The results of structural properties are in good agreement with the available theoretical data. Spin polarized band structure calculations predict the semiconducting nature of this compound along with a large energy gap. Ferromagnetic interactions among the constituent atomic spin moments determine the total magnetic moment μ= 3.01591 μB .The real and imaginary parts of dielectric function, refractive index, absorption coefficient and reflectivity are calculated.

Key words: DFT; Double perovskite; GGA+U; optoelectronic

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

CrYSi (Y= Be, Ra), a half-Heusler with half-metallic ferromagnetic properties: a DFT calculation.

Mahdjoub kheireddine zoubir[a], BLAHA Lamia Farah[a], KHATIR Radja[b]

[a] Laboratory Physico-Chemestry of Advanced Materials,University of Djillali Liabes;BP89,22000,Sidi Bel Abbés,Algeria
[b] Laboratory of Electrical Engineering and Materials (LGEM), Oran, 31000, Algeria

Abstract:

In the present work we have performed self-consistent ab-initio calculation using the full potential linearized augmented plane-wave method (FP-LAPW), based on the density functional theory (DFT) as implemented in the Wien2k code to study the structural, electronic, magnetic, thermodynamic and thermoelectric properties of the half-heusler compound **CrYSi (Y= Be, Ra)** using generalized gradient approximation (GGA) described by Perdew–Burke–Ernzerhof (PBE), GGA+U and the modified Beck-Johnson correction (mBJ) , the obtained results show that the compound is stable in the ferromagnetic state (FM) in phase on one hand and has a half-metallic character (metallic nature in spin up channel and semiconductor one in spin down channel with an indirect gap)on the other hand thus, the compound is a good candidate for spintronic applications, moreover it shows a very interesting thermoelectric predispositions in the minority spin or spin down channel at room temperature consisting of a very high Seebeck coefficient, high electrical conductivity and figure of merit near unity for the two compounds.The thermodynamic properties of CrBeSi and CrRaSi compounds using Gibbs code are studied for the first time. This study showed that these compounds can be used in extreme thermodynamic conditions. Since no experimental data were reported until now concerning this compound, our theoretical

predictions of electronic, thermodynamic and thermoelectric properties are likely to be experimentally verified.

Key words: Spin down; FP-LAPW; high Seebeck coefficient; Half -Heusler; Spintronic applications.

Corresponding Email: mahdjoub.kheireddine.zoubir@gmail.com

References

[1]. S. Wolf, D. Awschalom, R. Buhrman, J. Daughton, S. Von Molnar, M. Roukes, et al., "Spintronics: a spinbased electronics vision for the future," science, vol. 294, pp. 1488-1495, (2001).

[2]. T. Dietl, H. Ohno, F. Matsukura, J. Cibert, and e. D. Ferrand, "Zener model description of ferromagnetism in zinc-blende magnetic semiconductors," science, vol. 287, pp. 1019-1022, (2000).

[3]. J. Balluff, T. Huminiuc, M. Meinert, A. Hirohata, and G. Reiss, "Integration of antiferromagnetic Heusler compound Ru2MnGe into spintronic devices," Applied Physics Letters, vol. 111, p. 032406,(2017).

[4]. D. Kieven, R. Klenk, S. Naghavi, C. Felser, and T. Gruhn, "I-II-V half-Heusler compounds for optoelectronics: Ab initio calculations," Physical Review B, vol. 81, p. 075208, (2010).

[5]. S. Gupta and K. Suresh, "Review on magnetic and related properties of RTX compounds," Journal of Alloys and Compounds, vol. 618, pp. 562-606, (2015).

[6]. T. Graf, P. Klaer, J. Barth, B. Balke, H.-J. Elmers, and C. Felser, "Phase separation in the quaternary Heusler compound CoTi 1− x MnxSb–A reduction in the thermal conductivity for thermoelectric applications," Scripta Materialia, vol. 63, pp. 1216-1219, (2010).

[7]. S. Sakurada and N. Shutoh, "Effect of Ti substitution on the thermoelectric properties of (Zr, Hf) NiSn halfHeusler compounds," Applied Physics Letters, vol. 86, p. 082105, (200).

[8]. M. Katsnelson, V. Y. Irkhin, L. Chioncel, A. Lichtenstein, and R. A. de Groot, "Half-metallic ferromagnets: From band structure to many-body effects," Reviews of Modern Physics, vol. 80, p. 315, (2008).

[9]. R. De Groot, F. Mueller, P. Van Engen, and K. Buschow, "New class of materials: half-metallic ferromagnets," Physical Review Letters, vol. 50, p. 2024, (1983).

[10]. I. Galanakis, P. Dederichs, and N. Papanikolaou, "Slater-Pauling behavior and origin of the halfmetallicity of the full-Heusler alloys," Physical Review B, vol. 66, p. 174429, (2002).

P-191

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Removal of Copper from Industrial Wastewater by seeds of *Moringa*

KENICHE ASSIA[a], KHELASSI ASME[b], ABOURA AMINA[a], SOLTANI YASSEMINE IKRAM[a].

[a] Laboratory of Organic Chemistry Natural Products and Analysis, University of Tlemcen.
[b] Maghnia Center University, Departement of Hydraulic, 13000,Maghnia, Algeria.

Abstract: We picked as a characteristic adsorbent in this work the Moringa Oleifera Seeds (MOSs) from Mali assortment, which could be a practical and earth safe strategy for water sanitization. All examinations were directed at room temperature, and after being permitted to represent two hours, the examples were broke down utilizing the Atomic Absorption Spectrophotometer (AAS). The seeds of Moringa were set up by taking around 1 g of the seed squashed and blending it in with around 20 cm3 of water to be decontaminated in three distinct measuring utensils. **Result:** The different arrangements after filtration, indicated an expanded thickness in the amount of copper, which demonstrates the viability of the cleansing intensity of the seeds of MO. The best consequences of absorption were for 30 min of contact time. We had half copper evacuation. The impact of contact time is significant in biosorption investigations to decide the harmony time required for the take-up of metal particles by the MOSs. **Conclusion:** In this investigation, the MOS from Mali were demonstrated to be a proficient regular adsorbent material of copper from fluid arrangements. The limit of the MOS to evacuate copper relies upon numerous models as; plant assortment and states of examinations. Our examination is going on the investigation of evacuation parameters, for example, contact time, pH, temperature, molecule size, sorbent portion, and introductory metal fixation.

Key words: Copper, MoringaOleifera Seeds, ,Water purification, Sustainable development.

Corresponding Email:

References [1] Keniche Assia, Medical Technologies Journal, *4*, **2020**, Pages: 504-515.

P-192

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Investigation of $A_2AlAgCl_6$ (A=Rb, Cs) using first principles: Potential utilization in UV optoelectronics

Smain Mesbah [a,c] , T.Lantri[a,b] , Mohammed.Houari[a,b], B.Bouadjemi[b], A.Boucherdoud[a], A.Khatar[b], B. Belarbi[a], O. Hammadache [a], S.Bentata[b] and M. Matougui[b]

[a] *University of Relizane 48000, Algeria.*
[b] *Laboratory of Technology and of Solids Properties, Abdelhamid Ibn Badis University of Mostaganem 27000, Algeria.*
[c] *Laboratory Physico-chemistry of Advanced Materials, University of Djillali Liabes, BP 89, Sidi- Bel- Abbes, 22000, Algeria*

Abstract:

In this study, we have investigated the electronic and optical properties of $A_2AlAgCl_6$(A=Rb, Cs) using first-principles calculations based on the Wien2k code with the GGA-PBE and mBJ exchange-correlation functionals. We performed computations on the cubic structure of space group Fm-3m. The band structure, density of states, and optical properties of Cs2AlAgCl6 have been investigated. The investigation shows that Rb2AlAgCl6 and Cs2AlAgCl6 have excellent mechanical and thermodynamic stability. They also have direct band gaps of 4.25 eV and 4.20 eV, respectively. Thorough investigation of the optical properties, including the dielectric function, absorption coefficient, and reflectivity, confirms that the materials are well-suited for UV devices application. This study provides a fundamental reference for future experiments that attempt to confirm the effectiveness of the methodologies used in this study, and to use these important characteristics for practical purposes in the field of research.

Key words: FP-LAPW; DFT; Nonmagnetic; Optical application; UV devices.

Corresponding Email: smail.mesbah@univ-relizane.dz

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Exploring the Physical and Optoelectronic Properties of Co_2ZrZ Compounds: Insights from Computational Analysis and Thermoelectric Characterization

Mohammed.Houari[a,b,*], S.Mesbah[a,c], T.Lantri[a,b], B.Bouadjemi[b], A.Boucherdoud[a], A.Khatar[b], A.Akham[b], B.Belarbi[a], S.Bentata[b] and M. Matougui[b]

[a] *University of Relizane 48000, Algeria.*
[b] *Laboratory of Technology and of Solids Properties, Abdelhamid Ibn Badis University of Mostaganem 27000, Algeria.*
[c] *Laboratory Physico-chemistry of Advanced Materials, University of Djillali Liabes, BP 89, Sidi- Bel- Abbes, 22000, Algeria*

Abstract:

This work uses Wien2k to calculate the physical parameters of Co2ZrZ compounds (Z= Pb, Bi, and As). Cobalt (Co) and Zirconium (Zr) Hubbard parameters are calculated using the Anisimov and Gunnarsson method. Results show that Co2ZrBi and Co2ZrAs are metallic, but Co2ZrPb is semi-metallic. The ??-X-direction energy gap calculations yield 0.328 eV (GGA) and 1.102 eV (mBJ-GGA). In both spin channels, the Co-D-eg and Co-D-t2g states dominate the valence bands of Co2ZrBi and Co2ZrAs. Infrared transitions below 0.56 eV decrease electron mobility, although UV absorption increases. Space solar energy applications may use Co2ZrZ compounds because they absorb UV radiation and improve conductivity. Satellites and space missions may benefit from Co2ZrPb's UV absorption. The refractive index drops below one in the high-energy band, indicating "Super-luminescence". Plasmatic oscillations also affect optics. The BoltzTraP thermoelectric analysis of Co2ZrPb shows a predominance of P-type charge carriers, indicating good electrical conductivity and low resistance. Co2ZrPb is suitable for thermoelectric applications because its ZT values vary between 0.99 (at 50 K) and 0.84 (at 1500 K), which are close to unity.

Key words: full Heusler, thermoelectric properties, Wien2k, Super-luminescence, space solar energy

Corresponding Email: houari.mohammed@univ-relizane.dz

P-194

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Commande hybride glissant flou d'un système éolien à base d'une génératrice asynchrone à double alimentation

Izzedine Allali[a], Boubekeur Dehiba[b]

[a] Laboratoire IRECOM Université Djillali Liabes, de Sidi Bel-Abbes,Algérie

[b] Laboratoire IRECOM Université Djillali Liabes, de Sidi Bel-Abbes,Algérie

Abstract:

This work present a technique of fuzzy sliding mode control applied to the system of wind energy conversion equipped with a doubly-fed induction generator. This technique finds its strongest justification for model uncertainty problems by using a nonlinear control law. The goal is to apply this command to control the exchange of active and reactive power generated by the doubly-fed induction generator with the network acting on the rotor signals via a bidirectional converter. The numerical simulation results obtained show the growing interest of such a control in electrical systems.

Key words: doubly-fed induction generator, fuzzy sliding mode, oriented flux control, power control..

Corresponding Email: Azziz.allali46@gmail.com

OnLine

Communications

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

CASTEP investigation of structural, electronic, and optical properties of NiSb2O6

CHARIF Rania[1], and MAKHLOUFI Rachid[2]

Laboratory of Applied Chemistry (LCA), Department of Matter Sciences, Faculty of Exact Sciences and SNV, University of Biskra, P.O. Box 145, 07000, Biskra, Algeria. 1
rania.charif@univ-biskra.dz

Abstract

The aim of this work is a study of the structural, and electronic properties of the trirutile NiSb2O6. The quantum DFT approximation used for this work was applied on the cobalt antimonate oxide a trirutile structure with a space group P42/mnm (136) and crystallized in tetragonal structure, with unit-cell parameters: a = 0.466, c = 0.924 nm. Without needing to make physical measurements, the structural characteristic of a material can be investigated by optimizing the first-principles computation. By utilizing the CASTEP code based on the pseudo-potential plane-wave within Material Studio software. In this study, NiSb2O6's geometrical optimization was done using a semi-local generalized gradient approximation (GGA) with the Perdew-Burke-Ernzerhof (PBE) for exchange - correlation functional, PBE for solids (PBESOL), Perdew-Wang91 (PW91) and RPBE functionals, as well as the local density approximation (LDA-CAPZ). After optimization, both records of bandgap and DOS of NiSb2O6 to understand its electronic properties. The NiSb2O6's electronic properties were determined by examining the electronic band structure and density of states, which are determinants of NiSb2O6 as a narrow gap semiconductor with a direct band gap.

Keywords: Spinel, Density Functional Theory, CASTEP, Band structure, density of states, NiSb2O6.

.

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Title : L'influence du glucose sur le dépôt d'argent et la résistance à la corrosion de l'acier inoxydable austénitique 316.

Djedjiga Ben Abdesselam[a], Youcef Hadjali[a], Belkacem Korichi[a] et Nacer Zazi[a].

[a] Université Mouloud Mammeri de Tizi-Ouzou, Faculté génie de la construction, Département de génie mécanique (LMSE), B.P.17 RP Tizi-Ouzou, Algérie.

Abstract:

Les aciers inoxydables austénitiques se distinguent par des caractéristiques particulièrement intéressantes, telles que d'excellentes propriétés mécaniques, une résistance accrue à la corrosion généralisée, et un coût compétitif par rapport à d'autres métaux, élargissant ainsi considérablement leur domaine d'application. Cependant, malgré ces avantages, les aciers austénitiques restent vulnérables à la corrosion localisée dans des environnements biologiques. Dans le cadre de notre étude, nous avons effectué une comparaison entre deux méthodes de dépôt d'argent sur l'acier inoxydable 316 austénitique : la méthode autocatalytique utilisant un procédé électrochimique et la réduction de l'argent (Ag^+) par le glucose, ainsi que la méthode de galvanoplastie (dépôt galvanique) sans glucose. Nous avons examiné l'impact de la présence ou de l'absence de glucose dans la solution, sur la résistance à la corrosion de l'acier inoxydable 316 après le dépôt. Les analyses ont été réalisées au moyen d'observations microscopiques électroniques à balayage, ainsi que par le tracé des courbes de polarisation i=f(E) et Log i=f(E). Le dépôt d'argent à la surface de l'acier 316 s'est révélé bénéfique en améliorant son potentiel de corrosion et sa résistance à la polarisation. La présence de glucose dans la solution, quant à elle, a entraîné une diminution du potentiel de corrosion de l'acier inoxydable 316. Par ailleurs, le dépôt d'argent sur les surfaces des aciers

inoxydables a démontré des améliorations significatives dans les propriétés antibactériennes, anti-corrosion, ainsi que, la capacité de réparation des fractures, selon diverses références. En conséquence, cette approche pourrait être considérée comme le meilleur traitement pour les matériaux destinés aux conditions d'implantation et aux applications alimentaires.

Key words: électrochimie, argent, potentiel, galvanique, glucose.

Corresponding Email: djedjiga.benabdesselam@ummto.dz

References

[1] S. Varmaziar, M. Atapour, et Y. S. Hedberg, « Corrosion and metal release characterization of stainless steel 316L weld zones in whey protein solution », npj Mater Degrad, vol. 6, no 1, Art. no 1, mars 2022, doi: 10.1038/s41529-022-00231-7.

[2] M. Sumita, T. Hanawa, et S. H. Teoh, « Development of nitrogen-containing nickel-free austenitic stainless steels for metallic biomaterials—review », Materials Science and Engineering: C, vol. 24, no 6-8, p. 753-760, déc. 2004, doi: 10.1016/j.msec.2004.08.030.

[3] D. Landolt, S. Mischler, M. Stemp, et S. Barril, « Third body effects and material fluxes in tribocorrosion systems involving a sliding contact », Wear, vol. 256, no 5, p. 517-524, mars 2004, doi: 10.1016/S0043-1648(03)00561-1.

[4] A. S. González et al., « Functional Antimicrobial Surface Coatings Deposited onto Nanostructured 316L Food-Grade Stainless Steel », Nanomaterials, vol. 11, no 4, Art. no 4, avr. 2021, doi: 10.3390/nano11041055.

[5] B. Lorsbach et E. Schmitz, « Influence of test parameters of potentiodynamic current density measurements on the determination of the pitting corrosion resistance of austenitic stainless steels », Materials and Corrosion, vol. 69, no 1, p. 37-43, janv. 2018, doi: 10.1002/maco.201709602.

[6] L. R. Hilbert, D. Bagge-Ravn, J. Kold, et L. Gram, « Influence of surface roughness of stainless steel on microbial adhesion and corrosion resistance », International Biodeterioration & Biodegradation, vol. 52, no 3, p. 175-185, oct. 2003, doi: 10.1016/S0964-8305(03)00104-5.

[7] S. A. Bouaziz et A. Zanoun, « Comportement électrochimique de l'acier X2CrNiMo17-12-2 (AISI 316L) boruré utilisé comme implant », Matériaux & Techniques, vol. 99, no 7, p. 717-724, 2011, doi: 10.1051/mattech/2011119.

[8] M. Petala et al., « Silver deposition on stainless steel container surfaces in contact with disinfectant silver aqueous solutions », Applied Surface Science, vol. 396, p. 1067-1075, févr. 2017, doi: 10.1016/j.apsusc.2016.11.090.

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

zero-dimensional Modeling of Dielectric Barrier Discharge in Pure Carbon Dioxide

Mohamed CHENOUI [a*] , Hocine TEBANI [a], Djilali BENYOUCEF [a] , Nesrine LABDOUNI [a]

[a] Laboratoire Génie Electrique et Energies Renouvelables, Université Hassiba Benbouali de Chlef, Chlef, Algeria

Abstract:

Carbon dioxide (CO_2) is a major contributor to climate change and a significant product of many human activities, notably industrial manufacturing, a major goal in the energy field has been to chemically convert emitted CO_2 into valuable chemicals or fuels, The modeling of plasmas plays a crucial role in understanding and characterizing various plasma processes, in this study focuses on modeling the dissociation of carbon dioxide in a dielectric barrier discharge plasma reactor via a zero-dimensional kinetics model, called ZD Plaskin. The model includes the most critical plasma species and reactions for the CO_2 splitting, the results show the evolution of the density of several species as function of time to obtain better insight in the underlying mechanisms and understand the dominant reactions pathways in CO_2 conversion.

Key words:

Plasma chemical kinetic modelling, CO_2 conversion, Dielectric barrier discharge

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

E-pharmacophore modelling, virtual screening studies and in-silico ADME analysis for identify new anticancer compounds

Presenting salma boulahia, saida khamouli

Abstract:

DNA of high-risk HPV 16 and 18 has been found to be associated with nearly 90% cases of cervical cancer.The viral E6 and E7 genes of HPV are regularly maintained and expressed in cervical cancer. So, the functional inhibition of E6 can be a promising therapeutic target. In the present work, a six-point e-pharmacophore model (AADHRR) was built and used for virtual screening of a focussed library of 30120 compounds, which was downloaded from Pubchem database. The pharmacophore-based virtual screening filtered out top 8995 hits, based on fitness score. Molecular docking tool like GLIDE was used for ligand-based virtual screening in the HTVS (high-throughput virtual screening) mode as it is very fast and less computational power is required. 2030 compounds (based on dock score) obtained from HTVS docking were further filtered to 180 hits employing docking in standard precision mode, which is computationally less demanding than docking in extra precision (XP) mode. Finally, best ten hits were identified using docking in XP mode. .ADME QikProp results suggested that identified hits have druglike physico-chemical properties. Present work re-affirms the previous finding that E6AP binding pocketon E6 protein is druggable. These identified hits may act as new leads for inhibition of E6 against cervical cancer.

Key words: : Cancer, criblage virtuel, Pharmacophore, Docking, Dynamique moléculaire.

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Removal of Indigo Carmine by Mg/Al layered double hydroxide

Fatima BOUCIF[a✉], Fatiha BESSAHA[b], Samira ZIANE[c], Amine KHELIFA[d]

[a,b,c,d] Département des Sciences et Technologie, Laboratoire de Structure, Élaboration et Applications des Matériaux Moléculaires, Université Abdelhamid Ibn Badis, Mostaganem, ALGERIE

Abstract:

The textile industry discharges large quantities of wastewater with a major toxicity risk. Treatments already exist, such as adsorption on activated carbon, which is an effective but costly process. Anionic clays could be both economical and less polluting adsorbents. They are double layered hydroxides with high adsorption capacities. We were interested in the synthesis of layered double hydroxides based on Mg and Al by coprecipitation at constant pH. The resulting material was calcined at 500°C for 3 hours, and applied to the removal of a Carmine Indigo dye in aqueous solution. This study is favored at pH=6 and the equilibrium time was estimated at 2 hours with an initial concentration of 300 mg/L Indigo Carmine. Modeling of the adsorption isotherms shows that the Langmuir model is the most appropriate for describing the adsorption isotherm of Carmin Indigo dye on MgAl-500 material, with a coefficient of determination value greater than 0.99. The maximum quantity adsorbed is of the order of 452 mg/g. We were able to conclude that adsorption by HDL (MgAl-500) is an effective process for the removal of anionic and azo dyes.

Key words: Layered doubles hydroxydes, Adsorption, dye, pollutant.

Corresponding Email:
boucif78@yahoo.fr

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

The use of solar photovoltaic energy in the field of water treatment

Zineb BENSACI [1*], Hicham SIBOUKEUR [1], Soulef BENABDESELAM [1], madjeda RAMDANI[2]

[1]Laboratory *LGEEMS*, Faculty of Applied Sciences, Kasdi Merbah Ouargla University, Ouargla 30000, Algeria.

[2]Laboratory *LAGE*, Faculty of Applied Sciences, Kasdi Merbah Ouargla University, Ouargla 30000, Algeria.

Abstract:

The issue of water resources has become a prominent challenge in contemporary societies due to the combination of rapid population growth and industrial development. Despite water covering a significant portion of the Earth's surface, only a small fraction, less than 1%, is suitable for domestic and industrial purposes. Conventional desalination methods, which rely on fossil fuel-powered technologies, not only consume substantial amounts of energy but also have detrimental effects on the environment. Consequently, the exploration of affordable and environmentally friendly renewable energy sources has emerged as a promising alternative to power modern desalination processes. In this study, we focus on the utilization of concentrated solar energy facilities for large-scale water desalination, as the generation of electricity from solar energy holds great potential in this regard. Specifically, we examine the characterization of the primary component in the photovoltaic system, namely the photovoltaic panel.

Key words: desalination, renewable energy sources, solar energy, photovoltaic system, the photovoltaic panel.

ON-07

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Synthesis of $FePO_4$ modify by Nickel, and their application in organic synthesis

Benali Belgharri [a,b], Berrichi Amina [a,b] , Abbou Sarah [a,b], Hamiani Zohra [a,b] , Bachir Redouane [a,c]

[a] Laboratoire de Catalyse et Synthèse en Chimie Organique, Université de Tlemcen, département de chimie, B.P.119 Tlemcen 1300, Algérie
[b] Université de Ain Temouchent, BP 284, 46000 Ain Témouchent, Algeria
[c] Université de Tlemcen,1300 Tlemcen, Algerie

Abstract:

This work focuses on the synthesis and characterization of new materials which is used as a catalyst for the synthesis of heterocyclic molecules.
Our research has mainly focused on metal-phosphate materials the invention is to introduce a new transition metal in our starting material iron phosphate III (FePO4). These materials undergo heat treatments to increase their structure and activity under organic reactions.
Heterocyclic compound have long been considered fundamental structural elements in the field of therapeutic and pharmaceutical treatments. This is due to their ability to offer a wide range of possibilities to substitute atoms or groups within their ring-shaped structures, highlighting their diversity and adaptability [1]. Isoxazole, in particular, is a preferred structure that has a wide range of biological activities and pharmacological properties. It occupies a significant place in various psychotropic drugs and an important position in the pharmaceutical field[2].
The new materials obtained were characterized by different physicochemical analysis technique : DRX, IR, SEM, specific surface measurement by BET and UV-Vis
The new catalysts were used in the synthesis of isoxazole from the chalcone taking into account the adequate conditions of the reaction. Catalysts showed good activity in isoxazole synthesis.

Key words: Catalysts, $FePO_4$, heterocycle, Isoxazole.

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Prédiction de l'isotherme d'adsorption optimale : Comparaison des modèles linéaires et non linéaires.

Salima Attouti[1], Mourad Termoul[1], Mokhtar Benzekri Benallou[1],Baghdad Benabed Fatma[1], Benaouda Bestani[1], Noureddine Benderdouche[1]

Laboratoire de SEA2M, Université Abdelhamid Ibn Badis, BP 227, Mostaganem, Algérie.

Abstract:

L'adsorption d'un herbicide l'acide 2,4 dichloro phénoxy-acétique (2,4-D) par un charbon actif à partir d'une solution aqueuse sur un charbon actif a été étudiée et les isothermes d'équilibre ont été déterminées.

Les données expérimentales obtenues à des différentes concentrations initiales ont été analysées en utilisant cinq modèles d'isotherme, le modèle de Langmuir, Freundlich, Temkin, Dubinin-Radkuvsky et Redlich–Peterson.

Afin de déterminer la meilleure isotherme convenable, une fonction d'erreur a été employée pour évaluer les résultats par la méthode de la régression linéaire et la régression non linéaire.

Les résultats montrent que la méthode non linéaire pourrait être une meilleure façon d'obtenir les paramètres pour les cinq modèles étudiés et l'isotherme de Redlich–Peterson confirme l'isotherme de Langmuir par sa constante g qui égale à l'unité.

La capacité maximale d'adsorption est de 235,55 mg/g calculée à partir du modèle de Langmuir.

L'étude cinétique a montré que l'adsorption du 2,4-D est régie par une cinétique de pseudo-second ordre et l'étude thermodynamique montre que l'adsorption est endothermique.

En outre, la nature d'adsorption de 2,4-D a été déterminée à partir des paramètres d'isotherme, et elle est conclue que la physisorption est le mécanisme approprié de l'adsorption de 2,4-D le charbon actif.

Mots-clés : adsorption, charbon actif, herbicide, isotherme d'équilibre, analyse d'erreur

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Wear Behavior of Nb-V-Cr Alloyed High Manganese Steel

Souad AYADI[a], Ali HADJI1[a]

[a]Foundry Laboratory, Metallurgy Department, BADJI Mokhtar University Annaba, BP 12-2300, Annaba, ALGERIA.

Abstract:

Austenitic manganese steel is designed to resist wear by friction, abrasion or impact. This steel is used in mines, quarries, alluvial mining, the recycling industry, cement plants with extraction, crushing, grinding and screening operations [1]. For this steel, the mechanical characteristic mainly sought is the wear resistance [2]. The purpose of this work is to improve the abrasion resistance of manganese austenitic steel by adding alloying elements (Nb, V and Cr).The samples were melt in an electric arc furnace. The alloying elements are added in powder form in a well heated ladle beforehand. The samples obtained underwent a heat treatment at 1100 °C followed by quenching with water. Optical microstructural analyzes, SEM and EDS were performed to evaluate the effect of added elements. Hardness measurements and friction wear tests were also performed to determine the wear resistance of the samples studied. The microstructures obtained reveal an austenitic matrix plus carbides precipitated at the grain boundaries in the raw state of casting in considerable proportions relative to the base steel. After heat treatment, these carbides completely dissolved. In this case, the microstructure reveals the presence of two phases, one corresponding to martensite and the other to residual austenite. The hardness measurements show an improvement of this characteristic after the addition of Nb, V and Cr. The wear tests show a clear difference in weight loss as a result of the addition of the alloying elements to the base steel. In the as-cast state, the wear resistance is improved by two to four times. By consequence in the treated state, it is so important that wear has become very low. This study has greatly improved the wear resistance with a low level of alloying element hence the interest of this work.

Key words: Manganese steel, Alloying elements, Carbides, Hardness, Wear.

Corresponding Email: ayadisouad14@gmail.com

References

[1] S. Ayadi, A. Hadji, K. Hakan, and D. Selman, "Microstructure and wear behavior of a Cr-Mo-Nb alloyed manganese steel," *J. Mater. Res. Technol.*, vol. 9, no. 5, pp. 11545–11562, Sep. 2020, doi: 10.1016/j.jmrt.2020.08.048.

[2] Souad AYADI and Ali HADJI, "Effect of Chemical Composition and Heat Treatments on the Microstructure and Wear Behavior of Manganese Steel," *Int. J. metacasting*, 2020, doi: https://doi.org/10.1007/s40962-020-00479-2.

ON-10

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Title: Study of the properties of selenium monochalcogenides SnSe and ZnSe by ab-initio simulation

Amel GASMALLAH[1,*], moufida BOUKHTOUTA [1,2], selma TOUAM[1], GACEM MAROUA[1] ,Ibtissem BENDJEDIDE[1], ines CHAREF[1]

[1] *Chadli Bendjedid University (UCBET), El Tarf 36000, Département of Physics, Algeria, Faculty of science and technology, Physical Chemistry of Materials Laboratory (LPCM).*

[2] *Badji Mokhtar University, Annaba 23000, Département of Physics, Algeria, Faculty of Science, Radiation Physics Laboratory (LPR).*

Abstract:

For the purpose of studying the structural and electronic properties of the XSe (X: Sn, Zn) binaries compounds, we employed the first principles calculations based on density functional theory (DFT). We applied the full-potential linearized augmented plane wave (FP-LAPW) method as implemented in the Wien2k code. Chalcogenides materials have attracted the interest of the research world, because of their involvement in the manufacturing of optoelectronic devices operating in the visible domain and solar panels. Our work is a comparative study between two types of chalcogens: SnSe and ZnSe concerning the structural and electronic properties. We used both the WC-GGA and mBJ approximations to study the structural and electronic properties. The results obtained for SnSe and ZnSe were compared with the previous works and were very compatible with experimental values

Key words: *SnSe, ZnSe, DFT, FP-LAPW, Wien2K, WC-GGA, mBj*

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Title: Efficiency of a shallow geothermal heat exchanger with soil-atmosphere interaction for space heating and cooling in the city of MOSTAGANEM.

BELHAMIDECHE Kheira[a], LAREDJ Nadia[ab], Mustapha Maliki[ab], MISSOUM Hanifi[ab], Djihad Bennaceur[a] ,Mahi Eddine Brahimi[a]

[a] Laboratory of Construction, Transport and Environmental Protection LCTPE, University of MOSTAGANEM.

[b] Department of Civil Engineering, Faculty of Science and Technology, University of MOSTAGANEM.

Abstract:

Among the different renewable energy sources, shallow geothermal energy (SGE) is regarded as a promising source for heating and cooling buildings. New approaches have recently been developed, including energy geo-structures, in which SGE systems are used in combination with heat exchangers in the ground (GHE). The thermal performance of a SGE system depends on a number of factors including the type of GHE, its thermal characteristics and the thermal behavior of the surrounding soil. The main objective of this study is to evaluate the performance of the GHE system under field conditions, taking into account the energy and water balance at the soil surface.

A transient numerical model based on the finite element method using the "Comsol multiphysics" software is developed, taking as parameters the thermal properties of the site soil, the climatology of an Algerian region and the atmosphere-soil-heat exchanger interactions in order to define the actual surface temperature over an annual reference period and the energy transferred to the building for heating or cooling.

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Physical properties of Silver Gallium Telluride (AgGaTe2) for sustainable energy technologies applications: A Density Functional Theory Study

Gouasmia Wissem[a], Boudjaadar Djamel[b], Oumelaz Faycal[c], Nimiri Ouarda[d], Louati Nesrine[e], Chebouki Sonia[f]

[a,c,d,e,f] Department of physics, Higher normal school of technological education of skikda, Algeria

[b] Department of physics ,LRPCSI-University of august 20th 1955 skikda, Algeria

Abstract:

$AgGaTe_2$, also known as Silver Gallium Telluride, is a semiconductor that exhibits exceptional thermoelectric properties. It has the ability to convert thermal energy into electrical energy, and vice versa, with high efficiency and low thermal conductivity. This is attributed to a unique phenomenon known as emphanisis. This material can also be used in solar cells to convert solar energy into electricity. Due to these properties, AgGaTe2 has potential applications in sustainable energy technologies, specifically in the domains of heat energy harvesting and solar energy. These properties motivated us to carry out this study. In this present work, we study the structural, electronic, and optical properties of Silver Gallium Telluride in the framework of the DFT using wien2k code.for structural data we found that lattice constants are a=b=6.3151A° while c=11.99146A° which are in good agreement with experimental data and other theoretical calculations. we also calculated the band gap which was found to be a direct one at gamma point and it's about 0.781 eV .for optical properties Spectral dependencies of both real ε1 and imaginary ε2 components of dielectric function ε(ω) have been calculated.

Key words: Silver Gallium Telluride; AgGaTe2; Semiconductor;;Electrical energy; Emphanisis; Solar energy; Structural properties; Electronic properties; Optical properties.

Corresponding Email: wissem.gouasmia@enset-skikda.dz

References

[1] V. A. Elyukhin, *Statistical thermodynamics of semiconductor alloys*. Amsterdam Boston Heidelberg: Elsevier, 2016

[2] M. Ya. Rudysh *et al.*, "AgGaTe2 – The thermoelectric and solar cell material: Structure, electronic, optical, elastic and vibrational features," *Infrared Phys. Technol.*, vol. 111, p. 103476, Dec. 2020, doi: 10.1016/j.infrared.2020.103476.

[3] S. Adachi, *Properties of semiconductor alloys: group-IV, III-V and II-VI semiconductors*, 1. ed. in Wiley series in materials for electronic & optoelectronic applications. Chichester: Wiley, 2009.

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

SYNTHESE ET APPLICATION DES NANOPARTICULES

Asma Bahloul[a], Ali Benayahoum[a, b], Samia Bouakkaz[a]

[a]Département de sciences de la matière, Faculté de mathématique, informatique, et de sciences de la matière, Université de 08 mai 45, 24000, Guelma, Algérie
[b]Centre de Recherche Scientifique et Technique en Analyses Physico- Chimiques (CRAPC)

Abstract :

Dans notre travail, nous avons synthétisées les nanoparticules de cuivre avec une réduction chimique d'ions de cuivre $CuSO_4$, en utilisant le N_2H_4 comme agent réducteur, et l'extrait de thé comme agent stabilisant et réducteur secondaire sous irradiation par micro-onde. Le spectre DRX de la poudre obtenue montre que le produit est un alliage Cu/Cu_2O d'un rapport 40/60 et de taille cristalline moyenne de 29 nm et 32 nm respectivement. Les nanoparticules de cuivre non-oxydées (Cu^0) ont été produite par une réduction de Cu_2O par l'agent réducteur (hydrazine) sans aucune oxydation. Le spectre UV-Visible de la solution colloïdale de cuivre présente un pic caractéristique des nanoparticules de Cu à 578 nm. Selon les résultats d'adsorption-désorption de N_2, la surface spécifique des nanoparticules synthétisées est de 23,209 m^2/g. l'analyse MEB révèle que la distribution de taille des nanoparticules allant de 30 à 100 nm et la majorité des particules se situent entre 50 et 55 nm. Afin d'étudier le pouvoir catalytique et l'efficacité des nanoparticules de cuivre à dégrader des colorants azoïques et non-azoïques, nous avons utilisé des modèles de réaction de réduction de 08 colorants et nous avons choisis la spectrophotométrie UV-Visible pour le suivi des réactions catalytiques, le taux de dégradation est compris entre 42% et 98%.

Key words : nanoparticules de cuivre, micro-onde, activité catalytique, chimie verte, non-conventionnelle

Corresponding autor E-mail: basma2765@gmail.com

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Biosorption of an inorganic pollutant from aqueous solutions

Bendellaa Ramila Chahinez, Didi Amel[a], Rekkab Afaf[a]

[a]Authors' Chemistry, Separation and Purification Technology Laboratory, Abu Bakr Balkaid University, Algeria

Abstract:

Pollution caused by heavy metals is a public health problem that requires appropriate solutions from environmental protection authorities. Due to its biodegradability and non-toxicity [1], biosorption is a suitable method for the recovery of these pollutants in diluted industrial aqueous solutions, it is economic and ecological, based on the use of non-living biological materials [2], which allow the removal of metal species, compounds, and particles from a solution. This study optimized and described the biosorption of the metal, in particular lead Pb (II) on carob after characterizing and identifying this biosorbent by Fourier transform infrared spectroscopy and zero charge point. The biosorption of Pb^{2+} ions on carob were optimized by studying the effect of different operating parameters such as pH, temperature, mass of the biosorbent, and stirring speed. Modeling of the experimental results obtained made it possible to describe adsorption as an endothermic and spontaneous process and physisorption following an apparent second-order mechanism.

Key words: pb^{2+} ion, Carob, biosorption, kinetics, thermodynamics.

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Effect of the Magnetic Field on Heat Transfer in a Corrugated Channel

abdelaziz boumaiza 1, a *, Ould lahoucine cherif 2, b

[a]Laboratory of Applied Mechanics of New Materials – LMANM, Faculty of Sciences Technology University of May 8, 1945 Guelma, Algeria
[b]Laboratory of Applied Mechanics of New Materials – LMANM, Faculty of Sciences Technology University of May 8, 1945 Guelma, Algeria

Abstract:

The current study analyzes the impact of a uniform external magnetic field on the hydrodynamic and thermal behavior of ferrofluid flow in a wavy channel using three-dimensional numerical simulation. The wavy surfaces at the top and bottom of the channel are heated with constant temperature, while the non-wavy section of the channel is thermally insulating. In the wavy section, in a direction perpendicular to the main flow, a regular magnetic field is applied along the direction of the main flow. The study explores the influence of volume fraction, Reynolds number, and magnetic field strength on thermal behavior of the ferrofluid flow. The results indicate an increase in heat transfer on the top and bottom walls with an increase in Reynolds number and magnetic field strength.

Key words: Convective heat transfer, nanofluids, magnetic field.

Corresponding Email : azize2520@gmail.com

ON-16

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Thermodynamic and Thermoelectric Properties of Ternary Half-Heusler Alloy: Suitable for green energy applications

S. Terkhi*[a], Y. Bouldiab[a], Y. Sefir[a], F. Bendahma[a], S. Benatmane[a], R. Bentata[a], M. C. Terkhi[b] and M. A. Boudjeltia [a]

[a]Laboratory of Technology and Solid's Properties, Faculty of Sciences and Technology, Abdelhamid Ibn Badis University, B.O 227, 27000 Mostaganem, Algeria
[b]Faculty of Sciences and Technology, Abdelhamid Ibn Badis University, B.O 227, 27000 Mostaganem, Algeria

Abstract:

Half-Heusler alloys have been identified as a class of promising thermoelectric materials due to their unexpected high thermoelectric performance with merit factor value of unity or larger. In this perspective, we have investigated the structural, electronic, thermal and thermoelectric properties of Half Heusler alloy FeVSn using density functional theory as implemented in the wien2k code. As the exchange and correlation potential, we employed two approaches: the generalized gradient approximation (GGA) and GGA-Tran-Blaha-modified Beck-Johnson (GGA-TB-mBJ). The electronic properties show that FeVSn has a Half metallic character with an indirect band gap in spin-up (Γ→ X) equals to 0.654eV (GGA) and 0.447eV (GGA-TB-mBJ). The thermodynamic properties show that FeVSn can be applied in extreme temperature and pressure conditions. Moreover, this alloy is characterized by high values of the merit factor (ZT) (close to the unity) which make it promising candidate for thermoelectric applications suitable in green energy applications as environmentally friendliness technologies.

Key words: First-principle calculations, Thermodynamic properties, Electronic transport, Merit factor.

Corresponding Email: *sabria.terkhi@univ-mosta.dz*

ON-17

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Synthesis and characterization of rare earth based coordination polymers with succinic acid and 1,10-phenanthroline

Yasmine Cheddani, Roza Maouche, Sabrina Belaid and Belkacem Benmerad

Laboratoire de Physico-Chimie des Matériaux et Catalyse, Faculté des Sciences Exactes, Université de Béjaia, 06000, Béjaia, Algérie

Abstract:

Recently, rare earth coordination polymers (CPs) have attracted a lot of interest and are the subject of a great deal of work, because they form fascinating structures with 1D, 2D or 3D networks [1]. The interactions between metal ions in these compounds can be very efficient, leading to interesting applications in different fields, such as optic and magnetism [2].

In this context, a series of rare earth based CPs has been synthesized hydrothermally, with succinic acid and 1,10-phenanthroline as ligands. The compounds are obtained as single-crystals.

Structural resolution was performed on the holmium-based compound, while the isostructurality of the other compounds was verified by powder XRD.

The CPs correspond to the formula: $[Ln(suc)_{1.5}(phen)]_n$, with (Ln= Ho(1), Dy(2), Er(3), Yb(4); phen=1,10-phenantroline; suc=succinate).

The asymmetric unit is composed of one Ho ion, a molecule of phenantroline, and one-and-a-half molecules of succinate (fig1).

The study of the thermal behavior of the compounds obtained, carried out by thermogravimetric analysis (TGA), shows that the CPs remain stable up to 335°C.

The study of the photoluminescence properties of the Dy-based CP with excitation at λ = 310 nm, shows very good emission for this compound in the (400-900) nm range, with the appearance of all the peaks characteristic of Dy (fig2) [3].

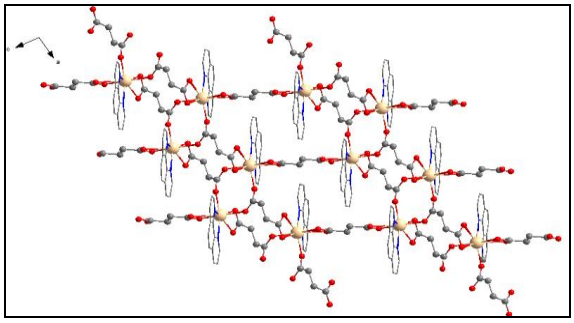


fig1: Projection of the structure along b axis.

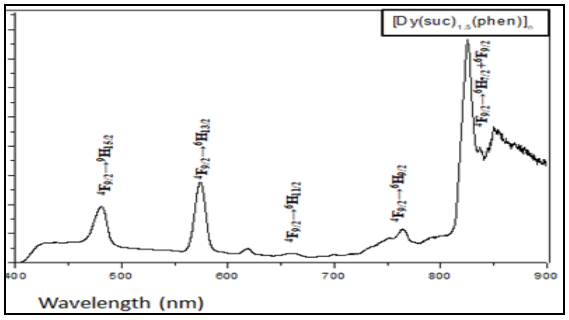


fig2: Emission spectra of Dy-based CP.

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Investigating $RbMgH_3$ Perovskite as Promising Material for Future Hydrogen Storage.

Sonia Chebouki[a], Ouarda Nemiri[a], Faycal Oumelaz [a], Boudjaadar Djamel[b]
Gouasmia Wissem[a], Louati Nesrine[a]

[a] Department of physics, Higher normal school of technological education of skikda, Algeria
[b] Department of physics ,LRPCSI-University of august 20th 1955 skikda, Algeria

Abstract:

The full potential linearized augmented plane wave (FP-LAPW) method framed within density functional theory (DFT) as realized in WIEN2k computational code is employed to explore the structural, electronic and optical properties of cubic peroviskite $RbMgH_3$. The optimization was performed employing generalized gradient approximation (WC-GGA) within the scheme of Perdew, Burke and Ernzrhof (PBE). The lattice constant of the optimized $RbMgH_3$ is 4.12 Å. The Perovskite type Hydride $RbMgH_3$ has an indirect band gap of 2.421 eV. As a result, at equilibrium, these compound exhibit semiconductor characteristic. The real and imaginary parts of the dielectric function are used to calculate the optical properties. Regarding hydrogen storage capabilities, the gravimetric hydrogen storage value $RbMgH_3$ compound is found to be 2.61 wt%. These computational analyses reveals that $RbMgH_3$ compound have a crucial role for hydrogen storage applications.

Key words: $RbMgH_3$, DFT, Gravimetric capacity, Hydrogen storage

Corresponding Email: chebouki.sonia@enset-skikda.dz

References

[1] Bayhan, Ü., & Yilmaz, İ. (2021). The structural, elastic, electronic, vibrational and gravimetric hydrogen capacity properties of the perovskite type hydrides: DFT study.

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Prediction of materials with high thermoelectric efficiency at high pressure

Maoudj Hanane

Abstract

The ultimate objective of this project is the proposal of new materials with high thermoelectric performance. The success in its achievement is associated with the fulfillment of two other intermediate objectives. The first is of a methodological nature and consists on the combination of prediction models of crystalline structures (XtalOpt, USPEX, …) with strategies for chemical-quantum calculation of electronic, thermodynamic and transport properties (VASP+newGIBBS). The second is of an applied nature. It seeks to obtain property-structure correlations from the computational exploration of regions of increasing pressures in the phase diagram of families of compounds with high value of the figure of merit (ZT) (AgCl, PbTe, SnSe, CoSb3) and allowing stoichiometric variations. The joint action of the computational tools and techniques along with their application is a unique opportunity to provide a better understanding of the parameters involved in ZT and advance in the rational design of materials that efficiently convert heat into electrical energy..

ON-20

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Title: Cocrystal Formation of the API Captopril with L-Arginine and L-Proline: Experimental and Theoretical Insights with DFT Analysis

Presenting author's : Omar elfarouk HOUACHE[a], Farida ALLAL[a] , Ali Benghia[a] Abdallah DAHMANI[b]

a. Mechanics laboratory, University Amar Telidji, BP37G Laghouat, Algeria
b. Laboratory of Thermodynamics and Molecular Modeling, Faculty of Chemistry, USTHB, BP 32 El-Alia, Bab-Ezzouar, Algiers, Algeria

Abstract:

This study explores cocrystal formation of captopril (CAP) with L-arginine (ARG) and L-proline (PRO) through the liquid-assisted grinding synthesis method. Differential scanning calorimetry (DSC), X-ray diffraction (XRD), Fourier-transform infrared spectroscopy (FTIR), and scanning electron microscopy (SEM) were employed for a comprehensive analysis, revealing distinct melting temperatures and eutectic compositions. Physical mixtures of CAP with arginine showed a simple combination of individual components, while the CAP-PRO system exhibited a new diffraction pattern, indicating a distinct cocrystal structure. FTIR spectra highlighted differences in wavenumbers, suggesting intermolecular interactions. SEM analysis revealed variations in crystal morphology between the CAP-PRO co-crystal and individual components. Additionally, theoretical studies employing Density Functional Theory (DFT) and Hirshfeld surface analysis, optimized coordinates via DFT, and calculated molecular orbital energies using the B3LYP functional were conducted. The Crystal Explorer software and GAUSSIAN 09 program were utilized for molecular Hirshfeld surfaces and visualization, respectively, offering valuable insights into the solid-state behavior and intermolecular interactions.

Key words: Cocrystals, L-arginine, L-proline, Captopril, DSC, XRD, FTIR, SEM, DFT, Phase diagram

Corresponding Email: o.houache@lagh-univ.dz

References omar elfarouk houache, farida allal , ali benghia abdallah dahmani, "Synthesis and Characterization of Captopril Co-crystals with L-Arginine and L-Proline," Pharm. Res., vol. 38, no.

ON-21

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

AB-initio study of the structural, electronic and optical properties of AlN and AlBi binary compounds by the Wien2k code

Monia ALAYAT[a], Selma TOUAM[a,b], Maroua GACEM[a], Ibtissem BENDJEDIDE[a]

[a] Department of Physics, Faculty of Science and Technology, Chadli Bendjedid University (UCBET), El Tarf 36000, Algeria.
[b] LPR Radiation Physics Laboratory, Department of Physics, Faculty of Sciences, Badji Mokhtar University, Annaba 23000, Algeria.

Abstract:

In this work, we systematically study the structural, electronic and optical properties of the binary compounds AlN and AlBi.

It is fair to say that III-V compound semiconductors play a crucial role in many advanced electronic and optoelectronic technologies. These materials are compounds formed by combining elements from group III and group V of the periodic table, such as (AlN) or (AlBi). Here are some of the applications you mentioned: High electron mobility and heterostructure bipolar transistors, Diode lasers, Light-emitting diodes (LEDs), Photodetectors, Electro-optic modulators, Frequency mixing components.

Key words: mBJ, FP-LAPW, optical properties, WIEN2K.

Corresponding Email:

alayatmonia@gmail.com

References

[1] M. Brikia, M. Abdelouhaba, A.Zaouib, M.Ferhata, Superlattices Microstruct. 4580(2009).
[2] P. Hohenberg, W. Kohn, Phys. Rev. 136 (1964) B864; W. Kohn, L.J. Sham, Phys. Rev. 140 (1965) A1133. W. Strunk Jr., E.B. White, The Elements of Style, fourth ed., Longman, New York,(2000).

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Ab initio investigations of the structure-stability, electronic, and magnetic properties of Cr-doped Na2S

Hemza MANCER[a], Habib RACHED[b]

[a]Hassiba Benbouali University of Chlef, Faculty of Exact-Sciences and Informatics, Laboratory for Theoretical Physics and Material Physics, Chlef, Algeria
[b]Djillali Liabes University of Sidi Bel Abbès, Faculty of Exact-Sciences, Magnetic Materials Laboratory, Sidi Bel-Abbès, Algeria

Abstract:

In this present work, we have used the full-potential augmented plane wave has been performed within the first-principles calculations of the framework of density functional theory and implemented in WIEN2K package to give estimated results of structural, electronic and magnetic properties of manganese doped alkali metal chalcogenide (Na_2S). The ground states were calculated and showed that the studies compound are energetically stable in ferromagnetic states. We have also calculated the formation energy (E_f) to affirm the thermodynamic stability at zero temperature and to analyses the alloying stability of compounds. therefore, we have found the negative sign of E_f parameter, confirming the favorable allowing stability of these compounds. The spin-polarized electronic structures including band structure and density of states are calculated employing the (GGA, GGA+U and GGA+U-mBJ). The analysis of the electronic structure reveals the excellent half-metallic ferromagnetic nature. The computed magnetic properties reveal that the total magnetic moment is generally attributed to the Cr atom with very small contribution from Na and S atoms. The obtained results from the important magnetic moment of these alloys indicate the potential for their use in spintronic devices.

Key words: DMS, Alkali metal, Cr doped, ab initio calculations

Elaboration and Characterisation of Mesoporous Materials. Study of Catalytic Properties.

Sadou Mohammed[a,*], Belabed Ahlam[a]

[a] Laboratory of Materials, Catalysis and Reactivity Chemistry (LCMCR), Hassiba Benbouali University of Chlef, B.O.Box 151, Chlef 02000. Algeria.

(*) Corresponding author: m.sadou@univ-chlef.dz

Abstract:

This work is based on a main objective concerning the improvement of the structural and textural properties of hexagonal-shaped M41S mesoporous materials (MCM-41) in the field of catalysis by insertion of a heteroatom in this case copper. It is established that the specific properties of a catalyst, resulting in its stability, strongly depend on the hydrothermal preparation method to develop the mesoporous copper-based silicate catalysts of different molar ratios (n = Si / Cu = 10 and 50) from a source of silica and a surfactant (CTAB). In order to better control the entire sequence of functionalization of materials, many characterization techniques have been used to qualify and quantify the species present on the surface. Therefore, the physico-chemical properties of the materials were established using the following techniques: DRX, IRTF, BET, SAA. In this study, we have considered the possibility of using MCM-41 type mesoporous materials as a catalytic support for the hydrogenation of benzaldehyde to benzyl alcohol.

Key words: mesoporous materials, MCM-41, hydrogenation, benzaldehyde, ...

References

[1] D. Haffad, U. Kameswari, M. M. Bettahar, A. Chambellan, J. C. Lavalley, J. Catal. 172 (1997) 91.

[2] M.Y. Ngai, J.R. Kong , M.J.Krishe ,J. Org. Chem., 72 (4) (2007) 1063–1072.

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Synthèse et hydrolyse du polyacrylamide .Caractérisation Etude des propriétés.

H. Briki[1], F. Metref[1].

[1] USTHB, Laboratoire des matériaux polymères, Faculté de Chimie, BP 32 El Alia, 16111 Alger, Algérie
[2] USTHB, Laboratoire d'hydrométallurgie et chimie inorganique moléculaire, Faculté de Chimie, BP 32 El Alia, 16111 Alger, Algérie

Abstract

Les polymères hydrosolubles tel que le polyacrylamide, peuvent jouer un rôle très important dans le domaine de la préservation de l'environnement. En effet, le polyacrylamide peut acquérir la propriété de polyélectrolyte par simple hydrolyse thermique qui lui permet une facile complexation avec les ions métalliques bivalents tel que Cu+2. Ainsi, le polyacrylamide neutre ou hydrolysé pourrait être utilisé comme purificateur d'eau polluée par les rejets industriels. Dans le cadre de cette communication, nous avons dans une première étape synthétisé et caractérisé par différentes techniques deux polymères (polyacrylamide) de masses différentes que nous avons hydrolysés en milieux aqueux neutre par simple chauffage thermique à 90 0C.Dans une seconde étape, nous avons réalisé les réactions de complexation de ces polymères avec un ions métallique bivalent Cu+2 dans les milieux acide, neutre et basique .Les complexes obtenus ont été analysés par spectroscopies infrarouge transformée de Fourier (FTIR), analyse thermogravimétrique (ATG), spectroscopie ultaviolet-visible, conductivité et potentiométrie. Enfin, les résultat obtenus, sont présentés et discutés dans cette communication.

ICMSE'2024

The 3rd edition of the International Conference on Materials Science and Engineering and their Impact on the Environment

Title: Predicting Damage in CFRP Bi-Graded Plates with Glass-Epoxy Materials

Mohamed El Amine Khiari[a], Fatna Telli[a]

[a] LaRTFM Laboratory, Department of Mechanical Engineering, National Polytechnic School of Oran Maurice Audin, BP 1523 EL M'NAOUER, Oran, Algeria

Abstract:

The use of composite materials has expanded due to their exceptional benefits across multiple industries, especially in the reinforcement of notched constructions. These continue to pique the interest of numerous researchers who want to improve them through analysis. The only way to examine their reinforcements indeed is to analyse their damage. It may take numerous pictures, such as geometric or material, complete or partial, at the notch's stat, depending on the suggested reinforcement. This work aims to completely reinforce the structure using the CFRP bi-graded glass-epoxy materials that have been suggested.

These three distinct fiber qualities combined to create a single quality in the center for each design case, by the suggested graduation design. This is acceptable as long as the fibers are contained in an epoxy matrix of the same grade and volume fraction. XFEM technique is used to homogenise the stiffness parameters and the graded damage in the structure according to thickness by volume fraction introduced by finite element analysis. To do this, a unique mesh is employed. The characteristics that were evaluated, including the kind and density of finite elements, the mesh architecture, the degree to which the parameters satisfied the damage criteria, and the introduction of these parameters, all had an impact on the results that were

reached. To achieve this, a specialized mesh is utilized, wherein the assessed parameters such as the type and density of finite elements, as well as the mesh architecture and its conformity with the damage criterion, all demonstrate an impact on the determined outcomes. The linear constitutive law employed in our model aligns with the Von Mises equivalent stress flow theory. The composite material utilized in this study is CFRP. Assessment of the graduation parameters' influence is conducted on the structure's response and its resistance capacity using tensile separation curves. The investigation revealed that in scenarios where the strongest fiber is positioned in the middle of the plate, there is a symmetrical distribution of stress relative to the structure's thickness, accompanied by an excess capacity in resistance.

Keywords: CFRP (carbon fiber reinforced polymer);FGM (functional graded materials); XFEM (extend finite element method); CZM (cohesive zone modeling)
Corresponding Email: Kh.mohamed1294@gmail.com

References

[1] Abdelouahed, E., Mokhtari, M., Habib, B., Ghermaoui, I. M. A., Ezzine, M. C. E., Ghomari, A., & Merasli, Y. (2023). Using a non-linear mixed model behavior of CZM to predict the damage in single lap bonded joint with bi-composite graded materials. *Mechanics of Advanced Materials and Structures*, 1-15.

[2] F. Telli, M. Mokhtari, M.E.A. Khiari, B. Habib, A. Slamene, and E. Abdelouahed, Damage analysis of hybrid carbon/glass-Epoxy pipe elbows under bending and pressure loading, Mech. Adv. Mater. Struct., vol. 30, pp. 1–17, 2023. DOI: 10.1080/15376494. 2023.2226953.

[3] F.Z. Messabih, M. Mokhtari, M. Bentoumi,A. Slamene, E. Abdelouahed, H. Benzaama, A. Ghomari, and Y. Merasli, Nonlinear czm-based predictive analysis of damage in single-lap composite joints: An exploration of the fgm concept in fiber– matrix coupling, Mech. Adv. Mater. Struct., vol. 30, pp. 1–11, 2023. pp. DOI: 10.1080/15376494.2023.2263974.

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Title: Optimization of a customized passive polyurethane foam mattress to optimize the human body's sleeping position

Abdelkader BENKHETTOU [a], Omar KHATIR [a], Ismail BOUDJEMAA [a], Abderahman SAHLI [a]

[a] Department of Mechanical Engineering, University of Sidi Bel Abbes, Laboratory Mechanics Physics of Materials (LMPM), Algeria.

Abstract:

The individual's posture plays a very important role in comfort, but there is no "ideal" position for lying on a mattress, although there are some recommended positions. However, as each individual has a unique physiognomy, the optimum mattress for each person needs to be personalized. The aim is to design and optimize a customized polyurethane foam mattress to ensure optimal posture and reduce the intervertebral shearing forces that act on the body when lying down. the mattress has been designed with 38 horizontal sections in the variable-rigidity polyurethane foam support layer. To obtain a personalized mattress for each individual, we used the Genetic Algorithm (GA) optimization to obtain an optimal configuration of the polyurethane foam segments in the support layer in order to obtain the best posture for the individual.

Key words: Mattress, sleeping position, Optimization, Customized Mattress, Polyurethane Foam.

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Ab intio investigation of electronic and magnetic properties of Ca_{1-x} TM_x Te (TM= V, Cr, and Mn).

Youcef Daoudi[a,b], Hadj Moulay Ahmed Mazouz[a,c], Mohamed abdelilah Fadla[d], Ali Benghia[d]

[a] Département de Physique, Faculté des Sciences, Université M'hamed Bougara, Boumerdes, 35000, Algérie
[b] Unité de Recherche Matériaux, Procédés et Environnement (UR-MPE), Université M'hamed Bougara, Boumerdes, 35000, Algérie.
[c] Laboratoire de Modélisation et Simulation en Sciences des Matériaux (LMSSM), Université Djillali Liabes, Sidi Bel Abbes, 22000, Algérie.
[d] Laboratoire de physique des Matériaux (LPM) , Université Amar Telidji de Laghouat, Route de Ghardaïa, B.P. 73G Laghouat, 03000, Algérie.

Abstract:

The interesting characteristics of spintronics exhibit lower energy consumption, higher density, push up us to find new materials that can be functional for spintronics such as half metallic ferromagnets. Based on density functional theory (DFT) and using full potential linearized augmented plane waves and local orbitals (FP-LAPW+lo) method implemented in Wien2k package, we carried out a study of structural, electronic and magnetic properties of CaTe doped with V, Cr, and Mn for various concentrations namely x=0.25, 0.125, and 0.0625. Tran-Blaha-modified Beck-Johnson potential (TB-MBJ) was used to investigate the electronic and magnetic properties. We found that: only Cr-doped compounds are half metallic ferromagnetic materials with 100% spin-polarisation at Fermi level (E_f) and their ferromagnetism stabilization is explained by Zener's double exchange mechanism. An integer integrated total magnetic moment per TM atom marked to be 3,4, and 5 in Bohr magneton(μ_B) for V, Cr, and Mn-doped compounds respectively. We found large half metallic gaps for Cr dopant compounds resulting from the strong p-d hybridization of 5p (Te) and 3d (Cr), which make them promising candidates for spintronic devices and applications.

Key words: Density functional theory, spintronics, half-metallic ferromagnets, diluted magnetic semiconductors, half-metallic gap, electronic and magnetic properties.

Corresponding Email:

daoudi.youcef.phd@gmail.com

ON-28

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Title: Conception of SPR-based sensor for cancer cell detection

Mohamed Esseddik Ouardi[a], Kada Abdelhafid Meradi[a], Fatima Tayeboun[b]

[a] Institute of Science and Technology, University of Ain Temouchent, BP 284, 46000 Aïn Témouchent, Algeria.
[b] University Djillali Liabes, 22000 Sidi-Bel-Abbès, Algeria.

Abstract:

In this study, a high-sensitivity surface plasmon resonance sensor (SPR) for the detection of cancerous cells is presented and analyzed, the BK7 prism, silver, gallium arsenide, and sensing medium are layered successively into the structure of the sensor. The sensing medium contains various cells. The geometrical parameters such as the thickness of the layers are modulated to reach high performance. The proposed SPR-based sensor has maximum sensitivity of 243 deg/RIU, a figure of merit of 39.5 deg^{-1}. These sensing abilities allow the suggested sensor to be a useful tool for identifying various cancer cell types. To analyze the performance parameters of the sensor, the structure is simulated using the transfer matrix method (TMM) on MATLAB.

Key words: SPR, Surface Plasmons, Cancer cell, Transfer Matrix Method, biosensing.

Corresponding Email: mohamed.ouardi@univ-temouchent.edu.dz

Introduction

ICMSE'2024

The 3rd edition of the International Conference on Materials Science and Engineering and their Impact on the Environment

Title: Using FGM to Predict Damage in carbon-Epoxy Composite

Fatna Telli[a], Mohamed El Amine Khiari[a], Elamine Abdelouahed[b], Mourad Chama[a] ,Mohamed Mokhtari[a]

[a] LaRTFM Laboratory, Department of Mechanical Engineering, National Polytechnic School of Oran Maurice Audin, BP 1523 EL M'NAOUER, Oran, Algeria
[a] LaBAB Laboratory, Department of Mechanical Engineering, National Polytechnic School of Oran Maurice Audin, BP 1523 EL M'NAOUER, Oran, Algeria

Abstract:

Reinforcement in composite structures has been a key focus for researchers, commonly addressed through hybrid composites or graded materials. This study explores a novel approach using finite element analysis and ABAQUS code to predict the performance of composites graded by a Functionally Graded Material (FGM) concept. Unlike conventional thickness-based grading, this method introduces volumetric fraction variation into Fiber-Matrix mixing laws in unidirectional composites. The study examines thickness-graded composites under thermomechanical loading, proposing three grading concepts (C-S, C-2, and C-3) with varying fiber density distributions. Results indicate enhanced resistance in graded composites compared to non-graded counterparts, particularly influenced by the grading index (n) and fiber distribution. Damage is primarily attributed to deformation overcapacity.

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Synthesis, characterization of the perovskite Eu-doped $KNbO_3$ and its application for hydrogen evolution under visible light

Romaissa MEKERSI[*1], *Souhila BOUMAZA* [1] *and Mohamed TRARI* [2]

[1]Laboratory of Chemistry of Natural Gas, Faculty of Chemistry (USTHB), BP 32, 16111 Algiers, Algeria.
[2]Laboratory of Storage and Valorization of Renewable Energies, Faculty of Chemistry (USTHB), BP 32, 16111 Algiers, Algeria.

Abstract:

Perovskite oxides (ABO_3) exhibit great potential in photocatalysis due to their distinctive structure, flexible composition and remarkable stability. These catalysts are crucial in the fields of energy storage, energy conversion and the photodegradation of organic pollutants [1]. The pursuit of alternative energy sources has become a matter of great importance. One promising and cost-effective strategy is the generation of hydrogen from water using semiconductor catalysts and sunlight. However, for this approach to be viable, the catalyst material needs to possess certain qualities such as: chemical stability, affordability and the ability to efficiently capture a significant portion of the solar spectrum [2].
In the present work, Eu-doped $KnbO_3$ was synthesized by the nitric combustion method and has been characterized by X-ray diffraction (XRD), attenuated total reflection (ATR), scanning electron microscopy (SEM) and diffuse reflectance spectroscopy (DRS). The XRD pattern obtained at 700 °C, showed a pure phase $KNbO_3$, crystallizing in the perovskite structure. The synthesized oxide has been successfully tested for hydrogen production under visible light.

Key words: Perovskite, $KNbO_3$, Photocatalysis, Hydrogen.

Corresponding Email:

mekersi.romaissa1997@gmail.com

ON-31

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Study Of The Physical Properties Of Binary And Ternary Compounds Based On Samarium (Sm)

Bendahah Abla[a], Bensaid Djillali[b], Bencherif Kaddour[c], Mokadem Khadidja[d] , Amrani Lemya[e]

[a]Department SM, Faculty of Sciences and Technology, UBBAT,LMM UDL SBA, Algeria
[b]Depertment GE, Faculty of Sciences and Technology, UDL SBA,LMM,UDL SBA, Algeria
[c]Department SM, Faculty of Sciences and Technology, UBBAT, LEMIO UDL SBA, Algeria
[d]Department SM, Faculty of Sciences and Technology, UBBAT, LMM UDL SBA, Algeria
[e]Department SM, Faculty of Sciences and Technology, UBBAT, LMM UDL SBA, Algeria

Abstract:

Spintronics is a new field of research that exploits both the quantum and magnetic properties of electrons. Ferromagnetic semiconductors based on rare earth oxides such as europium monoxide EuO or samarium monoxide SmO whose magnetism comes from partially filled 4f states. Doping with a d or f element makes it possible to increase T_C with a decrease in resistivity, and gives us a metal insulating transition induced by a change in band structure[1]. We are interested in the ferromagnetic half-metallic phase of this kind of compounds. We try to substitute SmO with transition elements such as Co, Sc, Ti and Cr an ab-inition study of the physical properties of doped SmO, SmS, SmTe and SmSe compounds was carried out using the pseudopotential method within the framework of density functional theory (DFT) with the approximations GGA, GGA+U and mbj

Key words: Doped semi conductor, DFT, spintronics, half- metal

Corresponding Email: abila_05@yahoo.fr

References

[1] Yutaka Uchida, Kenichi Kaminaga, Tomoteru Fukumura, PHYSICAL REVIEW B 03 **2017**,95, 125111.

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Ab initio investigations of the structure-stability, electronic, and magnetic properties of Cr-doped Na2S

Hemza MANCER[a], Habib RACHED[b]

[a]Hassiba Benbouali University of Chlef, Faculty of Exact-Sciences and Informatics, Laboratory for Theoretical Physics and Material Physics, Chlef, Algeria
[b]Djillali Liabes University of Sidi Bel Abbès, Faculty of Exact-Sciences, Magnetic Materials Laboratory, Sidi Bel-Abbès, Algeria

Abstract:

In this present work, we have used the full-potential augmented plane wave has been performed within the first-principles calculations of the framework of density functional theory and implemented in WIEN2K package to give estimated results of structural, electronic and magnetic properties of manganese doped alkali metal chalcogenide (Na_2S). The ground states were calculated and showed that the studies compound are energetically stable in ferromagnetic states. We have also calculated the formation energy (E_f) to affirm the thermodynamic stability at zero temperature and to analyses the alloying stability of compounds. therefore, we have found the negative sign of E_f parameter, confirming the favorable allowing stability of these compounds. The spin-polarized electronic structures including band structure and density of states are calculated employing the (GGA, GGA+U and GGA+U-mBJ). The analysis of the electronic structure reveals the excellent half-metallic ferromagnetic nature. The computed magnetic properties reveal that the total magnetic moment is generally attributed to the Cr atom with very small contribution from Na and S atoms. The obtained results from the important magnetic moment of these alloys indicate the potential for their use in spintronic devices.

Key words: DMS, Alkali metal, Cr doped, ab initio calculations

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

The effect of mini channel geometries of AlSi10mg aluminum alloy cooler on the flow and thermal characteristics

Chadi kamel [a], azzouz el amin[b]

[a] Research Center in Industrial Technologies CRTI, P.O. Box 64, Cheraga, 16014, Algeria
[b] University of Science and Technology of Oran, 1505 El M'nouar, Oran, Algeria

Abstract:

In the current work, we conducted a three-dimensional numerical study of the effect of the mini channel geometry cooler's shape on the flow and thermal properties. Thereby, three cases of mini-channel cooler are considered. The first case contains a fluid inlet at the top and a side outlet, the second case contains a side inlet and an outlet, while the third case contains two side inlets and one outlet. Particularly, we chose an AlSi10mg aluminum alloy micro-channel cooler for the three cases. A constant heat flow is applied to the bottom wall of the cooler, used with an Al_2O_3- water nanofluid of a volume Al_2O_3 nanoparticles concentration of 5% as a coolant. The flow and heat transfer were studied for Reynolds numbers ranging between 200 and 500.

Numerical results have showed that the physical properties of the nanofluid gave a good thermal performance for the cooler with two inlets and one outlet, especially when the Reynolds number was increased, and also gave a lower temperature on the bottom wall of the cooler compared to other cases, and it can be used to improve the thermal performance.

Key words: Nanofluid, mini-channel, heat transfer.

Corresponding Email:

k.chadi@crti.dz

References

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Docking Moléculaire et Pharmacocinétique Appliqués à Une Série D'hétérocycles Quinazoline et Quinoléine

Faiza Asli [a], Saida Khamouli [b], Imen Bensahbane [c]

[a.b.c]*Group of Computational and medicinal Chemistry LMCE Laboratory, University Mohamed Khider, Biskra, 07000, Algeria University Mohamed Khider.Laboratoire,*

Abstract:

Background: Cancer, the disease of pathophysiological alterations in the inherent process of cell division[1], has emerged as a significant disorder responsible for a large number of deaths year by year worldwide[2]. More than 19.3 million (19,300,000) new cancer cases were diagnosed and reported recently, leading to approximately 10 million deaths in 2020 based on the reported data[3]. The continuous emerging incidences of cancer worldwide that causes millions of deaths annually have generated the need and demand for developing potent pharmaceuticals for treating different cancers[4]. Fortunately, along with the progress in medicine and therapies, researchers have gradually comprehended the tumor pathogenesis in the cellular and molecular scale, thus have revealed more and more vital signaling pathways and key biological macromolecules including membrane receptors and kinases[5].With the development of computer tools over the past 20 years. Molecular modeling and more precisely molecular docking has very quickly entered field of pharmaceutical research. Quinazoline and Quinoline derivatives can exhibit fine results in treating cancer via several different mechanisms, such as blocking the cell cycle, inducing the cell apoptosis, inhibiting the vascular growth, stopping the cell migration and activating the immune responses[6] .EGFR enzyme involved in cancer disease.

Results : Our work consists of studying the inhibition of EGFR (1M17) with deferent inhibitors derived from quinazoline and quinoline by molecular docking.

We used the MOE software for the optimization of the ligands by the semi-imperial AM1 method The values of ligands L148 and L177 are the best ligands for inhibit the activity of 1M17 since it forms a stable complex with this enzyme by better binding to the active site. The results obtained show that the ligands L148 and L177 give weak interactions with the active site residues EGFR (1M17) which stabilize the complexes formed of this ligands, which gives a better binding at the level of the active site, and an RMSD of L148 [1,9563 Å] and of L177 [1,2483 Å]. [1, 9563, 1.2483] Å

Conclusions: Our studies are based on the calculation of interaction energies, the RMSD and the interaction distances between the inhibitors and the receptor. Depending on the results obtained, we can choose the best inhibitor which has a high affinity to bind with the enzyme. The results obtained show that the ten ligands L148, L177, L198, L140, L143, L138, L161, L150 L164, and L136 forming a complex with the receptor ID: 1M17, and which have the lowest energies Score compared to the molecule of reference, this shows that these complexes are more stable. They can be classified in the following order: L148 < L177 < L198 < L140 < L143 < L138 < L161 < L150 < L164 < L136. We conclude that the values obtained are considered perfect for the 10 ligands, and especially the ligands L148 and L177 are the best ligands for inhibiting the activity of 1M17 since it forms a stable complex with this enzyme by better fixation on the active site.

Key words: Docking, EGFR, Quinazoline , Quinoliène, MOE

Corresponding *E-mail :* *faiza.asli@univ-biskra.dz*
E-mail : *saida.khamouli@univ-biskra.dz*
E-mail : *imen.bensahben@univ-biskra.dz*

References

[1] 1.H.K. Matthews, C. Bertoli, R.A.M. de Bruin. Cell cycle control in cancer. Nat. Rev. Mol. Cell Biol. 2022, 23 (1), 74–88
[2] D. Hanahan. Hallmarks of Cancer: New Dimensions. Cancer Discov. 2022, 12 (1), 31–46.
[3] J. Ferlay, M. Colombet, I. Soerjomataram, et al. Cancer statistics for the year 2020: An overview. Int. J. Cancer 2021, 149 (4), 778–789.
[4] A. Desai, C. Scheckel, C.J. Jensen, et al. Trends in Prices of Drugs Used to Treat Metastatic Non-Small Cell Lung Cancer in the US from 2015 to 2020. JAMA Netw. Open 2022, E2144923
[5] Duan, Y.T.; Sangani, C.B.; Liu, W.; Soni, K.V.; Yao, Y. New promises to cure cancer and other genetic diseases/disorders: Epidrugs through epigenetics. Curr. Top. Med. Chem., 2019, 19(12), 972-994. http://dx.doi.org/10.2174/1568026619666190603094439 PMID: 31161992

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Properties of Self-Compacting Mortar Containing Glass and Brick Powder

Yasmina Bouleghebar[a], Bentchikou Mohamed[b],

a Material and Environment laboratory (LME), Faculty of Technology, University of Médéa, Algeria
[b] Laboratory of Mechanic Physics and Mathematical Modeling (LMP2M), Faculty of Technology, University of Médéa, Algeria

Abstract:

The construction industry has been one of the largest sectors in the world, it is responsible for the consumption of 40% of natural resource extracts [1] , for that reason solutions must be found to help minimize the environmental problems generated, due to both the negative impact on the environment and the excessive use of natural resources [2].

In that order, various strategies and methods have been followed to improve the sustainability of concrete in terms of reducing CO2 emissions and conserving non-renewable natural resources to develop green and ecological concrete [3] . These strategies consist of using industrial by-products such as waste from construction sites, building demolition and factory waste [4].

Although glass and brick as a global replacement has already been the focus of many investigations, there has been less study on the partial substitution of cement with glass & brick specifically in Algeria. The performance of glass and brick powder self compacting mortar in terms of hardened properties (compressive and flexural strength tests at the ages of 07, 14, 28 days, alkali-silica reaction (ASR), and high temperature strength tests of 90-day cured SCM) were studied.The results indicated that SCM with Glass Powder and Brick Powder have showed an improvement in compressive and flexural strengths, and alike with the curing age compared to the control SCM. he incorporation of 24% GP and 20% BP as a supplementary cementing material, could significantly decrease the ASR expansion; The

SCMs containing GP and BP demonstrate better performance in terms of high temperature strength resistance, whilst the water-cured samples had higher residual strengths.

Key words: Self compacting Mortar, waste glass, Brick powder, Alkali silica reaction (ASR), High temperature strength

Corresponding Email:
yasmineboulegbar.93@gmail.com

References

[1] S. C. Angulo, V. M. John, C. Ulsen, H. Kahn, and A. Mueller, "Separação óptica do material cerâmico dos agregados mistos de resíduos de construção e demolição," *Ambient. Construído*, vol. 13, no. 2, pp. 61–73, 2013, doi: 10.1590/s1678-86212013000200006.

[2] D. Matias and J. Brito, "Incorporação de adjuvantes em betões produzidos com agregados grossos reciclados de betão," *Repensar a Construção Vol.1*, no. December 2004, pp. 339–344, 2004.

[3] G. Long, Y. Gao, and Y. Xie, "Designing more sustainable and greener self-compacting concrete," *Constr. Build. Mater.*, vol. 84, pp. 301–306, 2015, doi: 10.1016/j.conbuildmat.2015.02.072.

[4] A. M. Falmata, A. Sulaiman, R. N. Mohamed, and A. U. Shettima, "Mechanical properties of self-compacting high-performance concrete with fly ash and silica fume," *SN Appl. Sci.*, vol. 2, no. 1, pp. 1–11, 2020, doi: 10.1007/s42452-019-1746-z.

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Molecular modulation of Falcarinol in Anethum graveolens herbal essential oil against anti-inflammatory activity

Abdelmadjid Saidani[1]*, Abdelaziz Berghioua[2], Nasser Belboukhari[1], Khaled Sekkoum[1]

[1]Bioactive Molecules and chiral separation Laboratory (BMCSL), PO Box 417, University of bechar, 08000, Algeria
[2] Chemistry and Environmental Science Laboratory (LCSE)Faculty of Exact Sciences, University Tahri Mohamed of Bechar, PO Box 417, Bechar, 08000, Algeria

Email:, saidani.abdelmadjid @univ-bechar.dz

Abstract

Today's researchers are interested in vital compounds extracted from aromatic oils of medicinal plants for use in medicine and cosmetic products. The grass of anethum gravolens is a plant that is widely used in ancient Egyptians and is a modern growing herb in the Mediterranean and Southeast Asia regions, This herb was harvested in the Tagit region, south-west of Algeria. The oil was extracted from it by the Clevinger device and the basic oil analysis at Gas chromatography-mass spectrometry Falcarinol in Anethum graveolens herbal base oil against anti-inflammatory activity was merged into the Molecular Operating Environment Programme (MOE) and showed good results against RMSD inflammation estimated at 1.37 and S -7.23 .

Keywords: Anethum graveolens, GC-MS, anti-inflammatory activity.

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Synthesis of NiO nanoparticles by the Pechini sol-gel method

Blizak Meriem Djanette [a], Bouchenak Ouahiba [a], Blizak Salah [b,c]

[a] Bioinformatics, Applied Microbiology and Biomolecules Research Laboratory (BMAB), University M'Hamad Bougar of Boumerdes, Algeria
[b] Department of physics, Faculty of sciences, University Mohamed Boudiaf of M'Sila, Algeria
[c] Materials, Processes and Environment Research Unit (URMPE), University M'Hamad Bougar of Boumerdes, Algeria

Abstract:

Nickel oxide (NiO) nanoparticles have attracted considerable attention due to their remarkable photocatalytic properties, particularly in the field of environmental remediation and water purification. These nanoparticles can catalyse oxidation reactions to degrade pollutants and exhibit antibacterial properties, thus contributing to water disinfection. This study focuses on the synthesis of NiO nanoparticles using the Pechini method, a versatile technique developed and patented by Mario P. Pechini in 1967. Nickel acetate was used as a precursor, followed by a thermal treatment at 450°C for 2 hours. The structural properties of the particles were characterised by X-ray diffraction (XRD). The photocatalytic activity of the NiO nanoparticles was evaluated by assessing the degradation of methylene blue under UV irradiation. The XRD results showed that the nanoparticles synthesised by the Pechini method exhibited superior homogeneity and crystallinity. The increased crystallite size contributed to the photocatalytic efficiency of the NiO nanoparticles, as it can minimise carrier recombination and increase the active surface area for photocatalytic reactions. The Pechini method stands out as a valuable approach for the synthesis of advanced materials, offering exceptional homogeneity, reduced processing temperatures and the ability to produce nanomaterial while maintaining economic viability.

Key words: NiO nanoparticles, Pechini method, photocatalysis

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

An experimental study to improve the efficiency of the solar still by adding stuffed tubes to the still basin

Naima Mekhloufi [1], Mohammed Mostepha Belhadj [1], Mouhamed Elbar Soudani [1], …

[1] Faculty of Mathematics and Material SciencesUniversity Kasdi Merbah, Ouargla, Algeria

Abstract:

Given the major problem that most countries suffer from, most notably Algeria, specifically the desert areas, in terms of water desalination and the scarcity of potable water, as a solution to this problem, this study presents a simple method for producing potable water, as it relied on a single-cline distillation device with an experimental installation. Simple and easy on the one hand. It is powered by solar energy, which is renewable and inexpensive energy. This study aims to improve the performance of the simple solar still and increase the efficiency of the simple still. We conducted an experiment using two distillers. The first we added improvements and the second we saw. We have painted the incense burner with matte black paint. We placed copper tubes on the evaporator of the first distiller and made a comparison between the first and the second. The experiment was conducted on specific days in April 2021 in the climatic conditions of the city of Ouargla. The experiment showed that the results of the improved distillation device were better than those of the control distillation device because the tubes had a good heat storage effect

Keywords: Solar Still, Water Desalination, Heat Storage, Solar Energy.

ON-39

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Well Thickness Dependent Rashba Parameter and Spin Splitting in a (100) Grown GaAs/AlGaAs Double Quantum Well

Melaab Loubna[a] and Saadi Lamari[b]

[a,b] Physics Department , Faculty of Sciences, Ferhat Abbas University Setif 1, Algeria.

Abstract:

In this work we study the changes in the spin properties of bound electrons, in a (100) grown GaAs/AlGaAs double quantum well, brought about by variations in the quantum well thicknesses when the system is subject to an external electric field. Our calculations show that the Rashba parameter and corresponding spin splitting depend quite sensitively on well thickness and electric field magnitude. Moreover, we break down the resulting Rashba parameter in each subband into its four components which are related to discontinuities of specific physical parameters at the different interfaces of our system. Our analysis clearly shows that the overall dependence of the Rashba parameter results from the combination of different factors which add up algebraically leading to counterintuitive non trivial cancellations.

Key words: Double Quantum Well, two-dimensional electron gas 2DEG ,Well-Thickness, Rashba Spin Splitting, Interface Contributions.

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Numerical investigated to predict the damage in composite beam under tensile load

Benchaib Nadia[a], Mechab Belaïd[b], Medjahdi Malika[c], Salem Mokadem[b]

[a] Department of Mechanical Engineering, LMPM, University of Sidi Bel Abbes, Algeria.
[b] Department of Mechanical Engineering, LMPM, University of Sidi Bel Abbes, Algeria.
[c] Department. Energies and process engineering, Laboratory APELEC, University Sidi bel Abbes, Algeria

Abstract:

A composite material can be defined as the assembly of several materials of different natures on a microstructural scale. Composites usually consist of a matrix in which reinforcements have been dispersed in a controlled manner[1-2].In this work, a three-dimensional finite element method it's used to predict the damage of the composite structure subjected to tensile loads. Our work involves investigating the effects of the fibre orientation, thickness and properties of composite plate. The Monte Carlo method is used to predict of the composite damage. It is concluded that the effect of properties is very important in defining the failure rate of composite structures.

Key words: Composite, Finite element method, Numerical analyses , Monte Carlo method.

Corresponding Email:benchaibnadia95@gmail.com

References

[1] Das M, S. Sahu a, D.R. Parhi .2021. Composite materials and their damage detection using AItechniques for aerospace application: a brief review, Mater. Today: Proc. Vol 44, Part1, 955-960.

ON-41

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Title: Development and Characterization of a Ternary Inclusion Complex for Improved Niflumic Acid Delivery

Zohra BOUCHEKHOU[a], Amel HADJ-ZIANE[b], Bachir BOUZID[c]

[a,b,c]Laboratoire de génie chimique ; département de génie des procédés ; faculté de technologie ; UNIVERSITE SAAD DAHLAB-BLIDA , B.P 270 Route de Soumâa – Blida , Algeria

Abstract:

Niflumic acid (NA) is a non-steroidal anti-inflammatory drug (NSAID) that has established benefits [1]. Nonetheless, it has poor solubility, bioavailability, and significant adverse effects [2]. Complexing NA with cyclodextrins (CDs) presents a promising strategy to improve its delivery by overcoming these limitations [3]. However, complexing CDs with low molecular weight drugs, such as NA, can be challenging and often results in low complexation efficiency [4]. To address these issues, this study investigates the development of a ternary inclusion complex of niflumic acid (NA) with 2-hydroxypropyl-β-cyclodextrin (2HP-βCD) and hydroxypropyl methylcellulose (HPMC), including the effect of converting NA to its sodium salt (NAs) on complex formation. The complex is prepared using two methods: co-evaporation solvent and freeze-drying. complexation efficiency (CE) and apparent stability constant (Ks) for each complex were determined through a phase solubility study. The complex was then characterized in the solid state using various physico-chemical analyses, including differential scanning calorimetry (DSC), X-ray diffraction (XRD), and proton nuclear magnetic resonance spectroscopy (1H-NMR). Furthermore, the dissolution profile of the complex was determined and compared with the row NA. The analyses confirmed the formation of the inclusion complex, providing evidence of drug-cyclodextrin interactions, amorphous drug state, enhanced solubility and dissolution profiles.

ON-42

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Title: Density functional theory and molecular docking study of a novel organic pyrrole-based material

SMATI Sabrina [a], BOUKABCHA Nouredine [a,b], MENAD Karima [a],CHOUAIH Abdelkader [a]

[a] process engineering department ,University Abdelhamid Ibn Badis Mostaganem, Algeria
[b] Chemistry Department, Faculty of Exact Sciences and Informatic, University Hassiba Benali Chlef ,Algeria

Abstract:

Pyrrole, a five-membered ring structure containing nitrogen, is widely encountered in various chemical compounds, including bioactive ones. The incorporation of different pharmacophores into pyrrole-based structures has led to the development of highly active compounds. In this study, we synthesized and characterized (2Z)-3-oxo-N-phenyl-2-[(1H-pyrrol-2-yl) methylidene] butanamide monohydrate using XRD single crystal analysis and theoretical DFT quantum chemical computations with the B3LYP/6-311G (d,p) basis set. Our analysis involved comparing XRD results with theoretical calculations, assessing geometric properties, and examining HOMO-LUMO energy levels and chemical reactivity descriptors. Molecular electrostatic potential was also computed using the same basis set. Furthermore, NCI-RDG analysis was conducted to evaluate non-covalent interactions within molecular systems, providing insights into intermolecular bonding. Finally, we predicted the compound's biological activity through molecular docking, examining the types of bonds involved. This comprehensive approach aimed to bridge experimental observations with theoretical insights, elucidating the synthesized compound's structural and electronic properties.

Key words: Pyrrole,DFT,FMOS,GCRD,RDG,MEP,docking

Corresponding Email: sabrina.smati.etu@univ-mosta.dz

ON-43

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Numerical Study of Ozone Generated by Dielectric Barrier Discharge in O_2-Ar Mixture

Nesrine Labdouni [a*], Djilali Benyoucef [a], Hocine Tebani [a]

[a] Laboratory of Electrical Engineering and Renewable Energies, Faculty of Technology, Hassiba Benbouali University of Chlef, Algeria

Abstract:

Arising from the increased concern with environmental protection, ozone attracts widespread attention as an important oxidizing agent, finding use in a wide range of industrial applications such as disinfection of water and atmospheric air [1]. It is a gas formed from three oxygen atoms that are highly reactive and unstable compared to oxygen. Ozone is generated through the three-body collision reaction shown in reaction $O + O_2 + M \rightarrow O_3 + M$ M, the third particle involved in the collision process, could in dry air be either O_2, O_3, N_2 or Ar [2]. Ozone can be generated by using a dielectric barrier discharge (DBD) generator, which is also one of the most efficient and low-cost methods [3].

A numerical model based on a dielectric barrier discharge in **O_2**-Ar mixtures at atmospheric pressure is developed in this study to investigate the influence of Ar addition on ozone generation. The discharge is generated by two dielectrics of relative permittivity of 9 and powered by a sinusoidal voltage of 6 kV at 3 kHz of frequency. The numerical model is developed with COMSOL Multiphysics software.

Key words:

Fluid Model, Dielectric Barrier Discharge, Ozone, Plasma, Argon, Atmospheric pressure

*Corresponding Email: n.labdouni@univ-chlef.dz

ON-44

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

DYNAMIC BEHAVIOUR OF CONFINED N-HEPTANE AND WATER IN BIFUNCTIONALIZED MESOPOROUS ORGANOSILICA SBA-15

Fekkar-Nemmiche Nadia.[a], Devautour-Vinot Sabine.[b], Silly Gilles.[b], Henn François[b], Mehdi Ahmed.[b]

[a] Ecole Normale Supérieure de Mostaganem. *.N° 7 Castors 27000Mostaganem . Algérie*

[b] *Institut Charles Gerhardt, Montpellier .France.UMR 5253 CNRS-UM2-ENSCM-UM1, PMDP, Pl. E. Bataillon, 34095 Montpellier cedex 05,*

Recently, periodic mesoporous organosilica (POMs) are known to be promising candidates for the use confinement of nanoparticle in adsorption and separation science, controlled release of drugs or antioxidants …etc. One of the major interests of the POMs is the possibility to functionalize the channel pores of the inorganic framework through the covalent coupling of an organic moiety to adjust their properties to different types of applications. The well-defined pore structure presented by SBA-15 material has made it very good candidate for fundamental studies at testing confinement for the characterization of porous solids.

Here, we report the detailed study of the dynamic and thermodynamic dynamic properties of n-heptane and water and confined in hybrid bifunctionalized SBA-15 materials, mainly focusing the impact of confinement on the behaviour of fluids (n-heptane and water) on the surface chemistry of nanapores investigated by spectroscopic and adsorption techniques.

First, the one-pot pathway of co-condensation method, which is characterized by simultaneous condensation of inorganic and organic precursors in a single step, is used to introduce phosphodiester groups in the mesoporous surface of SBA-15. The second modification inner of the surface pore is the trimethylsilylation of the silanols groups through the post-synthesis grafting of TMS groups.

The adsorption and conductivity of water and n-heptane confined in functionalized nanoporous silicas SBA-15 are studied by means of differential scanning calorimetry (DSC), complex impedance spectroscopy (CIS), and NMR experiments. The impedance spectra of all samples previously dried and then subjected to vapour pressure of water and n-heptane showed that the conductivity is connected to the transport of ionic charge while the ionic diffusion is not detected when the silica samples are dry. Adsorption and NMR experiments shows that the surface chemistry of the nanoporous SBA-15 modifies silica based properties from hydrophilic to hydrophobic.

Key words: nanoporous silica SBA-15, functionnalization, fluid confinement.

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

A Density Functional Theory Exploration of InAs/GaSb Superlattices for Optoelectronic Potential

Mansour Houda [a]

[a] Department of physics, University of Blida 1, Blida, 09000, Algeria.

Abstract:

In this paper, we conducted a theoretical investigation on the structural, electronic and optical properties of (InAs)m/(GaSb)n superlattices (m-n: 1-1, 2-2, 1-3 and 3-1), using the Full-Potential Linear Muffin-Tin Orbital (FP-LMTO) method in the framework of the theory of the Density Functional Theory (DFT) within the Local Density Approximation (LDA) technique, implemented in the code of calculation LmtART 7. The calculated electronic properties indicate that the SLs(m-n) monolayer number has a considerable influence on the band gaps. However, we have calculated and analyzed the total and partial density of states of (InAs)m/(GaSb)n superlattices, in order to determine their electronic behavior. Moreover, we have calculated the dielectric function ε(w), the refractive index n(w), the coefficient extinction K(w) and the reflectivity R(w) for radiation energies up to 35 eV.

Key words: Semiconductors, Optical properties, FP-LMTO, Superlattices.

Corresponding Email: mansourhouda48@gmail.com

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

2-thioxo -3N-(2-ethoxyphenyl) -5[40-methyl -30N-(20-ethoxyphenyl) thiazol-20(30H)-ylidene] thiazolidin-4-one: Growth, spectroscopic behavior, single-crystal investigation, Hirshfeld surface analysis, DFT/TD-DF computational studies and NLO evaluation

Amina lahouali dit yahyaoui[a], Merzouk saidj[a], Abdelkader chouiah[a]

[a] Laboratory of Technology and Solid Properties (LTPS), Abdelhamid Ibn Badis University of Mostaganem, Mostaganem, Algeria

Abstract:

A substance called 2-thioxo-3 N-(2-ethoxy phenyl-5[4-0-methyl-3 0N-(2-0-ethoxy phenyl) thiazol-2-0(3 0H)-ylidene] thiazolidine-4-one (E2Th2) was synthesized for this study. Its molecular structure was determined using IR, UV-Vis, and NMR spectroscopy, as well as single-crystal X-ray diffraction. Quantum chemical calculations were performed to better understand its structural, spectroscopic, and electronic properties, including HOMO and LUMO energy gap, MEP, and global reactivity descriptors. Theoretical calculations were performed using density functional theory (DFT) [1] based on the B3LYP/6-311G (d,p). The electronic transitions were calculated according to time-dependent density functional theory (TD-DFT). The analysis of HOMO and LUMO was used to determine the charge transfer within the molecule. The NLO [2] activity evaluation was based on the determination of the dipole moment, polarizability (α), first-order hyperpolarizability (β), and second-order hyperpolarizability (γ), which were calculated using the same level of theory. Additionally, The RDG and HS analyses revealed repulsive, attractive, van der Waals strong and weak interactions. The results suggest that the title compound has potential uses as a future NLO material**.**

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Ultrasound-promoted Elaboration of Novel Nanocomposites Based On a New Semiconducting Copolymer and Magnetite Nanoparticles Fe_3O_4: Application in Anionic Dye Adsorption

Massillia Ait Radi[a], Zakaria Cherifi[a,f] ,Bouhadjar Boukoussa[b,e] , Noureddine Karkachi [c] ,Younes Mouchaal[d], Khaldoun Bachari [f], Rachid Meghabar[a] and Nabahat Sahli[a]

[a]Laboratoire de Chimie des Polymères(LCP). Département de chimie.Université d'Oran 1 Ahmed Benbella, BP 1524, El-Mnaouer, 31000 Oran, Algeria.
[b]Laboratoire de Chimie des Matériaux (LCM). Département de chimie. Université d'Oran 1 Ahmed Benbella, BP 1524, El-Mnaouer, 31000 Oran, Algeria.
[c]Laboratoire de Microbiologie Appliquée (LMA). Département de biologie. Université Oran1 Ahmed Benbella, BP 1524, El-Mnaouer, 31000 Oran, Algeria.
[d]Laboratoire de physique des couches minces et matériaux pour l'électronique (LPCMME). Département de physique. Université Oran1 Ahmed Benbella, BP 1524, El-Mnaouer, 31000 Oran, Algeria.
[e]Département de Génie des Matériaux, Faculté de Chimie, Université des Sciences et de la Technologie Mohamed Boudiaf, El-Mnaouer, BP 1505, Oran, Algeria.
[f]Centre de Recherche Scientifique et Technique en Analyses Physico-Chimiques (CRAPC), BP 10 384, siège ex-Pasna Zone industrielle, Bou-Ismail CP, 42004 Tipaza, Algeria.

…

Abstract:

The current paper outlines the preparation of novel semiconducting nanocomposites based on a newly developed semiconducting copolymer poly(vanillin-co-thiophene) (PVTH) incorporated with different amounts of magnetite nanoparticles (Fe_3O_4 NPs: 3,6, and 9% by weight), via solvent casting method, assisted with ultrasonic irradiations. PVTH copolymer was obtained through the polycondensation of vanillin, a bioderived aldehyde, and thiophene, catalyzed with sulfuric acid. Fe_3O_4 NPs were synthesized using the coprecipitation method The structural, thermal, and morphological properties of the copolymer, nanoparticles, and the nanocomposites prepared were investigated using various analytical techniques.The samples

were evaluated in the removal of methyl orange (MO) from aqueous solution, for which different parameters and their effect on the adsorption efficacy were studied and discussed, including, the effect of adsorbent type, contact time, adsorbent mass, and initial MO concentration.

Key words: poly(vanillin-co-thiophene); Fe_3O_4 nanoparticles; novel nanocomposites; solvent casting method; Ultrasonic irradiations; methyl orange removal.

Corresponding Email: massilya08@gmail.com

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Study of The Inhibitory Efficiency on a Steel of Type API 5L X52

N. Meddah Araibi [1],*, M. Sadou1, M. Hadjmeliani[2]

[1]Laboratory of Materials, Catalysis and Reactivity Chemistry (LCMCR), Hassiba Benbouali University of Chlef, B.O.Box 151, Chlef 02000. Algeria.
[2] LPTPM, Hassiba Ben Bouali University of Chlef, B.O.Box 151, Chlef 02000., Algeria

Abstract

Corrosion is an automatic destruction of the metal due to its interaction with the surrounding environment; this phenomenon is a continuous process that cannot be eliminated easily. This is a process of great importance especially in view of their impact on the various industrial activities where the problem of corrosion has been taken into account for a long time. In this modest work, we propose to find a way to reduce corrosion of the API X52 steel sample and the use of green chemistry to extract a corrosion inhibitor from a «Datura Stramonium» plant at different concentrations in an aqueous solution of 1 mol/l chloridric acid (HCl). The study was carried out by the method of mass loss and electrical-potentio (change of current density as a function of electrical potential).

Keywords: corrosion, corrosion inhibitor, Stramonium Datura, X52, etc.

COMPUTATIONAL STUDY OF NEW PHTALIMIDO 1, 3-THIAZOLE DERIVATIVES AS CYTOTOXIC AGENTS FOR LEUKEMIA DISEASE

Imane Bensahbane[a], Nadjib Melkemi [a], Ismail Daoud [a, b], Asli Faiza[a]

[a] Group of Computational and medicinal Chemistry LMCE Laboratory, University Mohamed Khider, Biskra, 07000, Algeria
[b] Laboratory of Natural and bio-actives Substances. Tlemcen University Faculty of Science. P.O.Box 119-Tlemcen-Algeria

Abstract:

Acute lymphoblastic leukemia (ALL) is an aggressive malignancy distinguished by an inferior survival rate, especially acute lymphoblastic leukemia (Ph+ ALL), which is caused by the BCR-ABL protein produced in cells that contain the Philadelphia (Ph) chromosome and stimulates the bone marrow to produce an excessive number of lymphoblasts. The ABL1 kinase domain is a promising molecular target that has recently received immense attention for the development of cancer therapies. In this research work, a study of the cytotoxic properties of a series of phthalimido 1,3-thiazole derivatives toward two leukemia cell lines was carried out using a combination of different computational chemistry methods. A molecular docking/dynamics study was performed on a series of twenty-two phthalimido-1,3-thiazole derivatives against the BCR-ABL protein PDB code: 4WA9. Six of the best inhibitors were identified based on their energy scores. Referring to the results presented by MD simulation, these molecules form stable complexes with the protein. Several interactions are established between these molecules and the residues of the active site, namely H-donor and H-acceptor bonds and Pi-H interactions. These findings support the future role of phthalimido-1,3-thiazole derivatives against the ALL disease and may help to find a new therapeutic combination of drugs to treat relapsed acute lymphoblastic leukemia to improve overall survival.

Key words: Philadelphia-positive ALL, BCR-ABL, Molecular Docking/dynamic, ADME.

Corresponding Email: imane.bensahbane@univ-biskra.dz

ICMSE’ 2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Title: The influence of the green solvent on the synthesis yield

Wafaa BELACHEHEB[a], NAAR Nacira wife ABDELI[b], MEGHABAR Rachid[c], …

[a]Authors’ Department of chemistry, University of Oran1 Ahmed Ben Bella, Oran, Algeria
[b] Authors’ Department of chemistry, University of Science and Technology Houari Boumediene, Algiers, Algeria.
[c]Author’ s Department chemistry,University of Oran1 Ahmed Ben Bella, Oran, Algeria.

Abstract:

Text of the abstract

Green solvents are defined as friendly, non-toxic, and biosolvent (1). They play a crucial role in green chemistry, in which the fifth principle states that using auxiliary substances and solvents is necessary (2). In this paper, we propose a synthesis of green solvent based on Choline chloride and Oxalic acid dihydrate using the ultrasonic method. Different concentrations of these compounds are used to make a comparative study between each solvent in chemical synthesis. For this study, a biobased molecule was synthesized in the different green solvents prepared.

Key words: Green chemistry, Green solvent, Choline chloride, Oxalic acid dihydrate

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Title: Bismuth Ferrite as an efficient heterogeneous photo-Fenton-like catalyst for remediation of water contamination

Mohamed El Hadi BENSSASSI [a,b], Awatef DALI [b], Tahar SEHILI [b]

[a] Département de Chimie, Faculté des Sciences, Université 20 août 1955-Skikda, Algeria.
[b] Laboratoire des Sciences et Technologies de l'Environnement (LSTE), Faculté des Sciences Exactes, Université des Frères Mentouri Constantine 1, 25000 Constantine, Algeria

Abstract:

Heterogeneous Fenton catalysts are emerging as excellent materials for wastewater treatment and water depollution applications. In this work, we focus on the photodegradation efficiency of cresol red (CR), a cationic triphenylmethane dye, in the heterogeneous photo-Fenton-like system with bismuth ferrite (BFO) and oxalic acid (Ox) under NUV irradiation. The BFO catalyst was initially synthesized by a co-precipitation process and characterized by XRD, FTIR, and SEM-EDS to establish the crystalline composition and morphology. BFO or Ox alone was found to be unable to degrade CR under NUV irradiation (9.68% and 15.13 % after 120 min of irradiation, respectively); on the other hand, CR degradation was practically achieved by the BFO/Ox/NUV system (88.44%), which involved the creation of dissolved Fe-Oxalate. Kinetic profiles were evaluated under a wide range of experimental conditions in order to assess the effects of the initial concentration of oxalic acid, amount of BFO, and concentration of dyes. Excellent degradation rate was achieved with 1 mM of oxalic acid and 0.05 $g.L^{-1}$ of BFO. Chemical probe experiments indicates that hydroxyl radical (HO.) has major role for RC degradation. These results demonstrate that $BiFeO_3$ photo-Fenton-like catalyst may be an efficient approach for remediation of wastewater.

Key words: Bismuth ferrite, Oxalic acid, Cresol red, Hydroxyl radical, Heterogeneous Fenton.

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Evaluation of a Novel Polymer as a Bio-Coagulant for Fruit Juice Wastewater Treatment

Rafik MARIR[a], Khedidja BOUMAZA[a,b], Esma MAHFOUF[a,b], Zeynep BILICI[c], Nadir Dizge[c]

[a] Higher National School of Biotechnology Taoufik KHAZNADAR, nouveau Pôle universitaire Ali Mendili, Constantine, Algeria
[b] Biotechnology Laboratory, Higher National School of Biotechnology Taoufik KHAZNADAR, nouveau Pôle universitaire Ali Mendili, Constantine, Algeria
[c] Department of Environmental Engineering, Mersin University, 33343, Mersin, Turkey.

Abstract:

Fruit juice production industries require vast quantities of water. As a result, these sectors require suitable techniques to recycle the wastewater generated within the plant [1, 2].

In the current study, an exopolysaccharide (EPS) produced by a newly *Bacillus sp.* isolated strain, was extracted and characterized using Fourier transform infrared spectroscopy (FTIR). The effectiveness of this EPS as a bio-coagulant for treating fruit juice wastewater was evaluated by employing coagulation-flocculation process. The pH and EPS concentrations were varied, as these parameters were chosen for optimizing the treatment system. The FTIR study unveiled the presence of various functional groups, including hydroxyl and carbonyl groups. The optimum pH and concentration values for the biocoagulant were found to be 10 and 25 mg/L, respectively. The coagulation-flocculation process achieved final removal efficiencies for COD and turbidity, surpassing the results obtained with chemical coagulants.

In conclusion, our exopolysaccharide demonstrated remarkable effectiveness in treating fruit juice wastewater. This finding suggests the possibility of utilizing this EPS as a viable alternative in industrial wastewater treatment processes.

Key words: Exopolysaccharide, coagulation-flocculation, wastewater treatment, biopolymer.

ON-53

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Title: Optimization of pesticide adsorption conditions by intercalated halloysite: equilibrium isotherm study and modeling.

BELKACEM Fatima Zohra[a], AMAR Amine[b], KHELIFA Amine[c]

[a] Structure, Elaboration and Applications of Molecular Materials (SEA2M): Department of Process Engineering, Faculty of Science and Technology, University of Mostaganem, Mostaganem, Algeria.

[b] Structure, Elaboration and Applications of Molecular Materials (SEAMM), Department of Process engineering, Faculty of Science and Technology, University of Mostaganem, Mostaganem, Algeria.

[c] Structure, Elaboration and Applications of Molecular Materials (SEAMM), Department of Process engineering, Faculty of Science and Technology, University of Mostaganem, Mostaganem, Algeria.

Abstract:

Pesticides are pollutants found in wastewater due to the increase in agricultural activities over the years [1]. Their removal from wastewater is a major concern due to their high toxicity and mobility[2]. Currently, adsorption is one of the most widely used methods for their removal[3], in which modified clays are widely used.

The objective of this study was focused on the intercalation of the clay mineral halloysite. An organohalloysite was prepared using a novel procedure. Halloysite (H) was intercalated with a solution of an intercalating agent having a concentration equivalent to six times the CEC of the starting halloysite.

The material was characterized by various techniques (XRD, SEM). After intercalation and characterization, the nanohybrid and raw halloysite were used as a pesticide adsorbents, as a model molecule likely to be present in the environment. Adsorption was carried out. Various parameters were taken into account, namely pH, time, concentration and temperature. Kinetics were modeled according to the pseudo-first-order, pseudo-second-order and intra-

particle diffusion models. Isotherms were modeled using linear regression, through Langmuir and Freundlich models.

The best adsorbent underwent several adsorption/desorption cycles, in order to assess its regeneration capacity, with a view to its possible use on a larger scale.

Key words: Halloysite; intercalation; characterization; pesticides; adsorption.

Corresponding Email:

[a] fatimazohra.belkacem.etu@univ-mosta.dz

[b] amine.amar.etu@univ-mosta.dz

[c] aminekhelifadz@yahoo.fr

References

[1] S. Cosgrove, B. Jefferson, P. Jarvis, Environ. Technol. Rev. 8 (2019) 1 .

[2] Joshua O. Ighalo, Adewale.G.Adeniyi, Adedeji A.A, Recent advances on the adsorption of herbicides and pesticides from polluted waters: Performance evaluation via physical attributes, Industrial and Engineering Chemistry 93 (2021) 117–137.

[3] J. Salman, F. Hussein, J. Environ. Anal. Chem. 2 (2014) 2.

VALORIZATION OF VEGETAL BIOMASS BASED XYLANE

Boudjellal Djamel*[1], Maachou Hamida[2]and Madani Leila[1]

[1]Department of Materials Sciences/ Faculty of Sciences, University of Medea, Algeria
[2]Department of Nature and Life Sciences/ Faculty of Sciences, University of Medea, Algeria
Email: djamelboudjellal07@gmail.com

Abstract

Biopolymers play important role inmany applications, both for their biodegradability, their functional and nutritional properties and for their image as a product from acompletely renewable natural source. Among these biopolymers, xy lane are the most abundant non-cellulosic parietal polysaccharides in nature. It isalinear polymer , a back bone of D xy lopyranose units bonded in β-1,4, with irregular branching. The following work attempts to implement the proprieties, bioactivity and industrial valorization of this biopolymer .The first part contains the general concepts of xy lane . The second part deals with the different physicochemical and biological proprietie sof the xy lane molecule . The last part was devoted to the extraction processes and the applications of this macromolecule in bio energy, biogas and production of chemical products. Xy lane are known for their antioxidant, immunomodulatory, antitumor, anti diabetic, anticoagulant, and heap to protective activities. In addition, their hydrolysis into sugar sand platform molecules for the chemical industry of fersmore attractive recovery pathways.

Keywords: Xyl ane, Bio-polymer, Extraction, Biorefinery , Valorization.

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Eco-Friendly Synthesis of Biodegradable Plastics : A Study on PHB Production Using Locally Isolated *Bacillus sp.*

CHEBAHI Asma[a,b], MARIR Rafik[b], RIRA Moufida[b], ALALLA Affef [b]

[a] National Higher School of Biotechnology (ENSB), Department of Biotechnology, Biotechnologies Laboratory, Ali Mendjeli University City, BP E66 25100, Constantine, Algeria.
[b] National Higher School of Biotechnology (ENSB), Ali Mendjeli University City, BP E66 25100, Constantine, Algeria.

Abstract

Polyhydroxybutyrate (PHB) has garnered significant attention as an eco-friendly alternative to conventional plastics due to its biodegradability, renewability, and potential to reduce environmental pollution [1]. This study focuses on producing and characterizing PHB using the microbial fermentation processes of a locally isolated Bacillus sp. strain, demonstrating bioplastic-producing capabilities. The fermentation conditions were optimized to improve PHB's yield and purity. This involved adjusting the carbon sources (glucose, fructose, sucrose, glycerol, sodium acetate, and lactose) and nitrogen sources (malt extract, yeast extract, peptone, corn steep liquor, urea, $(NH_4)_2SO_4$, NH_4Cl, KNO_3, Na_2NO_2, NH_4NO_3) as well as their concentrations. The effects of time and physiochemical parameters such as temperature and pH were also considered. FTIR, NMR, DSC, TGA, and SEM were employed to assess PHB structure and composition. Results indicate that the highest amount of bioplastic, 1.03 g/L, was achieved utilizing glucose and yeast extract at a concentration of 1% and a temperature of 30°C for 72 h. The bio-based material's identity was established by the presence of hydroxyl, methyl, methylene, methine, and ester carbonyl groups and distinctive chemical shift signals identified by ^{13}C NMR and ^{1}H NMR spectra. PHB micrographs revealed a moderately porous material with a strong tendency to form an interconnected network. The polymer was thermally stable up to 240 °C, and DSC analysis

revealed a melting temperature of 293.6 °C. In summary, these findings underscore the potential of the locally isolated *Bacillus sp*. strain for sustainable bioplastic production, offering promising avenues for eco-friendly polymer synthesis and applications.

Key words: Polyhydroxybutyrate, Bioplastic, Eco-friendly, *Bacillus sp*, Biodegradability.

Corresponding Email : asmachebahi.ac@gmail.com

References

[1] E. Hernández-Núñez, C.A. Martínez-Gutiérrez, A. López-Cortés, Ma.L. Aguirre-Macedo, C. Tabasco-Novelo, M.O. González-Díaz, J.Q. García-Maldonado, Physico-chemical Characterization of Poly(3-Hydroxybutyrate) Produced by Halomonas salina, Isolated from a Hypersaline Microbial Mat, J. Polym. Environ. 27 (2019) 1105–1111. https://doi.org/10.1007/s10924-019-01417-y.

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Title: Elaboration and characterization of pure CuO, pure ZnO, and ZnO/CuO nanocomposite

Boughanem mohd oulmessaoud[a], Touka nassim[b], Mokhtari salim[c],

[a] Department of physics, Bouira university, Algeria
[b] Department of physics, Bouira university, Algeria
[c] Department of physics, Bouira university, Algeria

Abstract:

In this study, pure CuO, pure ZnO, and ZnO/CuO nanocomposite with a ratio of 70% ZnO and 30% CuO were successfully prepared by the sol-gel method and were deposited on glass substrates by spin coating. Various characterization techniques, such as X-ray diffraction analysis (XRD) and UV-Vis spectroscopy, were used to investigate the crystal structure and optical properties. The XRD results showed that the crystal structure of ZnO is hexagonal, and that of CuO is monoclinic. The particle sizes of 18.06nm, 12.88 nm, and 15.24 nm were consecutively measured for pure ZnO, pure CuO, and 70%ZnO/30%CuO. The result of UV-Vis spectroscopy indicates that the band gap energies of 3.25 eV, 1.43 eV, and 3.09 eV were respectively calculated by the Tauc method for pure ZnO, pure CuO, and 70%ZnO/30%CuO.

Key words: pure CuO, pure ZnO, Nanocomposite, sol gel, XRD

Corresponding Email:
m.boughanem@univ-bouira.dz

References

[1] Mohammed, E. A. (2022). Effect of Annealing on Sensing Properties of ZnO: CuO Nanocomposite Thin Films by the Sol-gel Method. *NeuroQuantology*, *20*(2), 32.

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Valorization of Eucalyptus camaldulensis inner and outer barks for biopolymer applications

Nacera Benouadah[a], Andrey V. Pranovich [b]

[a] Research Unit, Materials, Processes and Environment (UR-MPE), M'Hamed Bougara University, Algeria
[b] Laboratory of Natural Materials Technology, Wood and Paper Chemistry, Åbo Akademi University, Porthansgatan 3-5, 20500 Turku, Finland

Abstract:

Bark wastes today are viewed as a high-value resource for biopolymer applications due to their chemical richness and diversity. This work presents a comprehensive chemical characterization of the inner bark and the outer bark of Eucalyptus camaldulensis cultivated in Algeria.
The extractives were first isolated with an Accelerated Solvent Extractor (ASE) and then analyzed by Gas Chromatography-Mass Spectrometry (GC-MS). The content of pre-extracted bark in cellulosic polysaccharide and free sugar monomers was determined by Gas Chromatography (GC). The hemicellulose composition and amount was determined after the acid methanolysis and GC. The amount of lignin was determined gravimetrically by the Klason lignin method and the acid soluble lignin was determined by the UV method. Formic and acetic acids in the bark were determined by HPLC after alkaline hydrolysis.
It was found that the extractives content were similar in the outer bark (0.85%) and the inner bark (0.88%). The cellulose content was higher in the outer bark (33.4%) than in the inner bark (28.7%). Lignin and the total hemicellulose contents were more abundant in the outer bark (31.7, 26.2%) than in the inner bark (28.6, 19.3%) whereas, sugar monomers were more abundant in the inner bark (4.4%) than in the outer bark (3.8%). The variation in acetic and formic acids and ash contents between the outer bark (1.5, 0.006 and 2.5%) and the inner bark (1.3, 0.005 and 2.4%) was small. The obtained results showed that the bark can be considered a suitable feedstock for lignocellulosic biopolymer applications and also for the extraction of bioactive compounds that can be used in different sectors.

Key words: biopolymer; Eucalyptus camaldulensis; inner bark; outer bark; waste.

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Title: Synthesis of nanotubes based on tartaric acid

Guettai hakima[a], Sebaa fatima zohra[b], Sebti houari[c]

[a]guettai hakima' physical chemistry, exacte and applied science, Ahmed Ben Bella Oran1,Algeria.
[b] sebaa fatima zohra' physical chemistry, exacte and applied science,Ahmed ben Bella Oran1, Algeria.
[c]sebti houari' physical chemistry, exacte and applid science, Ahmed Ben Bella Oran1,Algeria.

Abstract:

Text of the abstract The synthesis of nanotubes based on tartaric acid is an exciting area of research in nanotechnology and materials science. Tartaric acid nanotubes are characterized by their nanometric tubular structure and their electroconductive properties, which makes them very promising for various applications. The synthesis of tartaric acid nanotubes begins with the preparation of reagents. The main reagents are, a tartaric acid monomer and an oxidizing agent, such as sulfuric acid (H2SO4) or a doping salt such as ammo nium persulfate. We characterized the nanotubes using various techniques, including scanning electron microscopy (SEM), infrared spectroscopy (IR), X-ray diffraction. The objective of this study is to determine the adsorbent power, to eliminate a cationic dye methylene blue in an aqueous medium

Key words: nanocomposites,naturalspolymer,nanotube ,dye methylene blue

Corresponding Email:

guettai 82hakima@gmail.com

References

[1] L. Zhang, M. Wan, Adv. Funct. Mater. 13 (2003) 815.
M.J. Kim, Y.D. Liu, H.J. Choi, Chem. Eng. J. 235 (2014) 186.
M. Adachi, T. Harada, M. Harada, Langmuir 16 (2000) 2376.
B.J. Kim, S.G. Oh, M.G. Han, S.S. Im, Langmuir 16 (2000) 5841.
W. Wu, D. Pan, Y. Li, G. Zhao, L. Jing, S. Chen, Electrochim. Acta 152 (2015) 126.
[2] L. Zhang, Y. Long, Z. Chen, M. Wan, Adv. Funct. Mater. 14 (2004) 693.
Z. Zhang, Z. Wei, M. Wan, Macromolecules 35 (2002) 5937

ON-59

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Elaboration of phosphor powders $Lu_x Gd_{1-x}PO_4$ doped with Pr^{3+} by sol gel method

Benarbia Meriem[a], HAMROUN Mohammed Salah Eddine [a,b], ARABECH Khadidja [a], …

[a] Macromolecular Research Laboratory, Faculty of Sciences, Abou Bekr Belkaid University, Tlemcen, Algeria
[b] Centre de Recherche Scientifique et Technique en Analyses Physico-Chimiques CRAPC, BP 384, Zone Industrielle, Bou-Ismail, 42004 Tipaza, Algeria

Abstract:

This work concerns a study the optical and structural properties of $LuGdPO_4$ doped with rare earths Pr^{3+}in the form of trivalent ions, this material has excellent properties, high luminous efficiency, fast decay time and good radiation hardness.

The obtained material was realized the sol-gel method, for different percentages of 'Lu^{3+} (x = 10%, 20%,30%,40%). The calcination temperature of nano powders and the formation of single-phase ($LuGdPO_4$) are estimated at 1000 °C.

The phase identification of samples was examined using X-ray diffraction (XRD). The morphology of the powders was studied through scanning electron microscopy (SEM). Infrared spectra were recorded using a Fourier transform infrared (FTIR) spectrometer.

Key words: Rare Earths, $LuGdPO_4$, Scintillator, Sol-Gel

Corresponding Email:

meriemarbia02@gmail.com

References

[1] Jan Kappelhoff , Markus Haase , Thomas Jüstel ,On the energy transfer from Pr^{3+} to Gd^{3+} in nanosized $LuPO_4$ particles, https://doi.org/10.1016/j.jlumin.2021.118418

[2] Xin-Yuan Sun , Yu Liu , Xiao-Lin Liu , Ren-Ping Cao , Yu-Nong Li , Liang-Wu Lin, Substitution of Y^{3+} for Gd^{3+} on the luminescent properties $BaGd_2O_4$:Eu^{3+} scintillating phosphors, http://dx.doi.org/10.1016/j.optmat.2014.03.044

Title: Synthesis and characterization of Nanocomposite of aniline and 2-chloroaniline by polymerization in-situ

Bouabida Nour El Houda,

[a]bouabida nour El houda ,Common Core , Science and Technology Organisation university of Mustaphastambouli Mascara, Country Algeria.

Abstract:

This research investigates the synthesis and characterization of a novel nanocomposite achieved through in-situ polymerization of aniline and 2-chloroaniline. Employing a range of analytical techniques, we meticulously examine the structural, morphological, and functional aspects of the nanocomposite. Our study illuminates promising pathways for the advancement of materials science, offering insights into the potential applications of these nanocomposites in electronics, sensing technologies, and biomedical fields.

The nanocomposites were prepared via In-Situ emulsion polymerization in different molar ratio in presence of exchange montmorillonite.

The nanocomposite were characterized by FTIR,UV and DRX and VC all this was confirmed the formation of Nanocomposites.

Key words: Nanocomposite , in-situ, aniline, 2-chloroaniline, vc

ON-61

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Fabricate a triboelectric nanogenerator from SnO2 co-doping fluorine and aluminum

Kazi Tani Mohammed Yacine[a], ElAssad Zemallach Ouarri Kada[b], Regis Barille[c], Benchouk Kheireddine[a]

[a] University Ahmed Ben Bella Oran 1, department of physics, laboratoire physique des couches minces et matériaux pour l'électronique, Algeria
[b] University Mustapha Stambouli Mascara, department of physics Institute, laboratoire physique des couches minces et matériaux pour l'électronique, Algeria
[c] University Angers/UMR CNRS 6200, MOLTECH-Anjou, France

Abstract:

Les nanogénérateurs triboélectriques (TENG) [1] sont des dispositifs qui convertissent l'énergie mécanique en énergie électrique en utilisant le phénomène triboélectrique [2] a l'aide du frottement. Ils sont souvent utilisés pour alimenter des capteurs et des composants électroniques à faible énergie [6]. Pour la fabrication des TENG on doit utiliser des matériaux spécifiques. Dans cette étude nous avons utilisé le co-dopage du SnO2 : F : Al [3] le dioxyde d'étain, un composant inorganique avec des propriétés physiques et chimiques uniques notamment ses propriétés semi-conductrices avec une faible résistivité électrique, afin d'améliorer les propriétés de la couche mince, elle nous donne une conductivité électrique qui peut être modulée en fonction de divers paramètres, ce qui le rend un composant polyvalent dans son genre. On a choisi le co-dopage du SnO2 : F : Al [3] par la technique spray pyrolyse [4] afin d'améliorer les propriétés de la couche mince, elle nous donne une conductivité électrique qui peut être modulée en fonction de divers paramètres, ce qui le rend un composant polyvalent dans son genre. De plus, le dioxyde d'étain est également utilisé dans l'industrie du verre pour améliorer la conductivité électrique [5] et la résistance aux rayures des substrats en verre, notamment dans la fabrication de panneaux solaires et d'autres composants électroniques.

Key words: Nanogénérateurs, spray pyrolysis, couches minces, substrat, SnO_2

Corresponding Email: kazitani.mohammed@edu.univ-oran1.dz

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Facile Preparation of a Supported Copper-modified HMS.

O. Zekri[a], T. Djelloudi[a]

[a] Department of applied organic chemistry, Institute of chemistry, USTHB, Algeria.

Abstract:

In recent decades, metal nanoparticles (MNPs), with small particle sizes, have drawn increasing attention as an important class of nanocatalysts because of their superior activities in heterogeneous catalytic reactions [1]. To overcome the problem of the poor stability and severe aggregation in catalytic processes, MNPs are immobilized onto solid supports [2]. Among all used supports, nanoporous materials, such as zeolites, mesoporous silica, and metal–organic frameworks (MOFs), with high surface areas have proven to be a class of ideal hosts to confine small MNPs in their nanopores. In the present study, a copper containing ordered mesoporous material 1%Cu-HMS, was synthesized by wet impregnation method and deeply characterized. The studied catalyst exhibited Langmuir type IV isotherms with a H1-type hysteresis loop that is characteristic of a typical long-mesoporous material with 1-D cylindrical channels and showed large BET surface area of 765 $m^2.g^{-1}$. The crystalline size of the CuO species, calculated by applying the Scherrer equation, is about 3,3 nm.

Key words: CuO, HMS, nanomaterials, nanocatalysts.

Corresponding Email: ouardiazekri@yahoo.fr

References

[1] L. Liu, A. Corma, *Chem. Rev.* **2018**, *118*, 4981.

[2] E. D. Goodman, J. A. Schwalbe, M. Cargnello, ACS Catal. 2017, 7, 7156.

ON-63

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Empirical model for masonry infill under lateral loading throught extensive database

Messas Amar[a], Adjrad Arezki[a], Benyahi Karim[a], Bouafia Youcef[a]

[a] Department of Civil Engineering, University Mouloud Mammeri Tizi-Ouzou, Organisation, Algeria

Abstract:

Reinforced concrete frames with masonry infill are widespread in Algeria. The behaviour of the masonry infill remains neglected in the analysis of these structures. This study proposes to evaluate the resistance of the masonry infill, based on a large experimental database collected from the scientific literature, containing 160 tests of reinforced concrete frames with masonry infill under lateral loading. Through multiple regression analysis and Student's t-tests, the parameters influencing the strength and stiffness of masonry infill under lateral loading are determined, and various equations are then proposed to predict the strength and stiffness of masonry infill.

Key words: Empirical model, Multiple regression analysis, Experimental database, Reinforced concrete Frame, Masonry infill

Corresponding Email: messas.amar.1@gmail.com

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Title: Adsorption of asphaltenes in presence of nanoparticles

Naamoun Karima[a], Daaou Mortada [b,], bounaceur boumediene[c], Ghalem Ikram [d]

[a]NaamounKarima' Physical Chemistry, Exact and Applied Sciences , Oran 1 Ahmed Ben Bella ,Algeria
[b]Daaou Mortada ' ,Industrial chemistry, Chemistry, University of science and Technology Oran (MB) , Algeria
[c]'Bounaceur boumediene, Physical Chemistry, Exact and Applied Sciences , Oran 1 Ahmed Ben Bella ,Algeria
[a]Ghalem Ikram' Physical Chemistry, Exact and Applied Sciences , Oran 1 Ahmed Ben Bella ,Algeria

Abstract:

The Aggregation of asphaltènes in crude oil is one of the major problems affected oil extraction, their ability to flocculate, adsorb on surfaces and form solid deposits. Nanoparticles with good catalytic properties are an attractive subject for the heavy oil industry. Metal oxide nanoparticle can provide highly dense surface groups with a high tendency for strong interaction and would quickly remove asphaltene from heavy oil and therefore making the remaining fraction of oil transportable for conventional processing. In this study, we focused on studying the effect of NiO nanoparticles on the aggregation sites of asphaltene molecules in dispersing media through the UV visible spectrophotometry method, the nanoparticles prepared by precipitation method and we also studied some of their properties as a preliminary step by fourier transform infrared spectroscopic (FTIR), DRX, MEB. For last, the performance of metal oxide nanoparticle evaluated as inhibitors of the asphaltene aggregation through adsorption experiments, were carried out at different initial concentrations of asphaltènes. The effect of the following variables on the quantity of adsorbed asphaltenes were studied, namely the contact time the initial concentration of asphaltenes, the temperature, the kinetics and the adsorption isotherms of asphaltenes have been modified by the different models.

ON-65

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Title: Synthesis of superabsorbent biopolymer and its applications

Hafida ZERIGUI[a], Rachide MEGHABAR[b], Fatima Zohra ZEGGAI[c]

[a]Authors' Department of chemistry, University of Oran1 Ahmed Ben Bella, Algeria
[b] Authors' Department of chemistry, University of Oran1 Ahmed Ben Bella, Algeria
[c]Author's Center for Scientific and Technical Research in Physico-Chemical Analyzes, Algeria

Abstract:

Text of the abstract

Alginates are polysaccharides considered as biopolymers, extracted mainly from brown algae. They are widely used in various fields and many industries because of their biocompatibility and biodegradability (1). In recent years, alginate hydrogels in the presence of divalent or trivalent cations (Ca^{2+}, Ba^{2+}, Pb^{2+}, Ti^{2+}, Fe^{3+}, Al^{3+}) have attracted many researchers due to its amazing properties and its medical and biomedical applications, as an active ingredient in skin dressings or as excipients (2).

In this paper, we propose a method for the synthesis of superabsorbent alginate hydrogels based on differents concentrations of iron oxide and titanium oxide using the sonicator. This ultrasound ensures good agitation between the molecules with possible speed adjustment. After that we dried hydrogels by two different methods (freeze dryer and oven). this allows us to make a comparative study between iron and titanium, the concentration of metals, and the difference between the use of the oven and the freeze dryer and their influence on the hydrogels using different methods of analysis: X-ray diffraction (XRD), Fourier transform infrared (FTIR) spectroscopy and Differential scanning calorimetry (DSC). Finally, to reinforce the work we have done we have done different application tests to study the effect of each sample.

Key words: Superabsorbent, Biopolymer, Hydrogels, Alginate

ON-66

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Simulation of a Vehicle Suspension System Using two Control Strategies

Amina KHETTAR[a], Anis DEBBACHE[b], Nadhira KHEZNADJI[c]

[a]Mechanical and Production Construction Department, Faculty of Mechanical Engineering and Process Engineering, University of Sciences and Technology Houari Boumediene, Algeria
[a]Mechanical Construction Department, Faculty of Technology, University of Boumerdes M'hamed Bougara
[b]Mechanical and Production Construction Department, Faculty of Mechanical Engineering and Process Engineering, University of Sciences and Technology Houari Boumediene, Algeria
[c]Mechanical and Production Construction Department, Faculty of Mechanical Engineering and Process Engineering, University of Sciences and Technology Houari Boumediene, Algeria

Abstract:

The quality and development of the suspensions guarantee better comfort and greater safety for passengers. Consequently, it makes one vehicle more attractive compared to another; to meet these requirements, several types of vehicle suspension controls exist, among this types which are approved and applied widely are Sky-Hook and Ground-Hook controls. So, in this work, we were interested in the study of a semi-active suspension system of a quarter vehicle model with two degrees of freedom, controlled by these strategies. With the aim of achieving the modeling, design, optimization and reliability of vehicle suspension systems, by evaluating the behavior of our model as well as the technical feasibility of these controls. A simulation was carried out under the MATLAB/SIMULINK environment of these strategies are compared with those of the semi-active system.

Key words: Simulation by MATLAB, Sky-hook control, Ground-hook control, Semi-active Suspension System.

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Nickel nanoparticles-decorated graphite-modified screen printed electrode toward the electrochemical determination of dopamine

Fatima Zahra Makhlouf[a], Mohamed Lyamine Chelaghmia[a], Azzedine Makhlouf[b], Maxime Pontié[c]

[a]Department of process engineering, University May 8, 1945 Guelma, Laboratory of Industrial Analysis and Materials Engineering, Algeria
[b]Department of process engineering, University Abbes Laghrour Khenchela, Algeria
[c]Department of chemistry, University of Angers, Group Analysis and Processes, France

Abstract:

In the last decade, material science saw major strides, notably in nanomaterials, prized for their remarkable properties like high surface area and electron conductivity. They find applications in medicine, electronics, and more, particularly in the advancement of electrochemical sensors [1]. Electrochemistry offers user-friendly, potent analytical methods, promising high-performance devices in medical diagnostics. Researchers have crafted numerous electrochemical sensors, including modified screen-printed electrodes, addressing human health needs and public demand effectively. Dopamine (DA), an electroactive neurotransmitter derived from L-Dopa, regulates reward, coordination, and mood. However, imbalances can lead to Parkinson's, Schizophrenia, and Alzheimer's diseases, affecting neurological functions [2]. In this paper, we demonstrate that SPE decorated with nickel nanoparticles was successfully used to determine dopamine with a high selectivity, wide linear responses and a low determination limit of 0.9 µM using DPV technique. The fabricated sensor was characterized by FE-SEM, EDX and AFM measurements and it was successfully employed for the analysis of DA in blood serum.

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Experimental Investigation on Improving Refrigeration Systems Performance Using Phase Change Material

Abir Abboud[a], Zakaria Triki[a], Rachid Djeffal[b]

[a]1Laboratory of Biomaterials and Transport Phenomena, University of Medea, Medea 26000, Algeria
[b]Unité de Recherche Appliquée en Energies Renouvelables (URAER) Centre de Développement des Energies Renouvelables (CDER), Ghardaïa 47133, Algeria

Abstract:

Refrigeration systems play a pivotal role in various sectors, including food preservation, medical storage, and climate control. However, conventional refrigeration technologies often entail high energy consumption and environmental impacts, prompting the exploration of innovative approaches to enhance system performance while minimizing energy usage. In this paper, an experimental study was conducted to assess the enhancement of a refrigeration system's performance utilizing a phase change material (PCM). The study involved an experimental refrigeration/freezing cell employing PCM as a thermal storage system to enhance heat transfer from the evaporator. The methodology involved comparing two scenarios: the first, testing the system with water (melting point 0°C), and the second, testing it with a PCM (melting point -10°C), with a programmable thermostat (-15°C), monitoring internal and external temperature changes, and energy consumption values. Depending on the type of PCM and thermal load, an improvement in storage time during power outage from approximately 14 hours and 18 minutes to 23 hours and 45 minutes was observed with water compared to the PCM. In addition, the energy consumption was approximately 17.1% to 18.9% lower with water compared to the PCM. Finally, the analysis of the results with ethylene glycol confirms that, the conservation time is increased almost twice as much compared to water-based PCM.

Novel α-sulfamidophosphonates analogues of Fotemustine: Efficient synthesis using ultrasound under solvent-free conditions

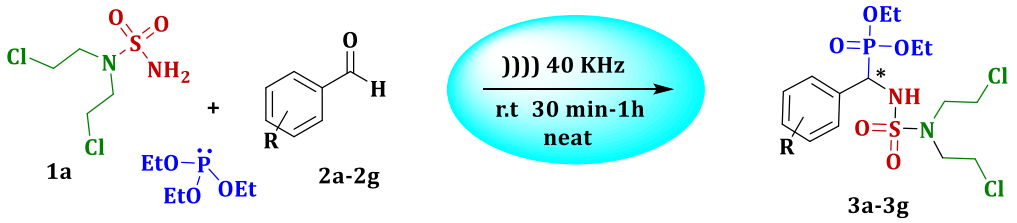
Guerfi Meriem[a], Boughaba Sara[b], Malika Berredjem[c], Christelle Marminon[d]

[a] Department of Pharmacy, Faculty of Pharmacy, University of Algiers 1 Benyoucef Benkhedda, Algeria
[b] Higher National School of Forests, Khenchela, Algeria
[c] Laboratory of Applied Organic Chemistry, Synthesis of Biomolecules and Molecular Modelling Group, Sciences Faculty, Chemistry Department, Badji-Mokhtar - Annaba University, Box 12, 23000 Annaba, Algeria.
[d] Faculty of Pharmacy-ISPB, EA 4446, University Lyon 1, Bioactive Molecules and Medicinal Chemistry, SFR Santé Lyon-Est CNRS UMS3453-INSERM US7, CEDEX 8, 69373 Lyon, France

Abstract:

The synthesis and reactivity of sulfonamides have aroused a lot of interest in recent years due to their important biological properties.[1] On the other hand, molecules with an amidophosphonate group have a very broad spectrum of biological activities. Among the many examples cited in the literature, we have found compounds which have shown potent antiviral activities against TMV, thus the proline derivative is an angiotensin inhibitor used as an antihypertensive agent.[2,3] One of the powerful tools used to connect economic features with the green concerns is performing organic reactions under ultrasound irradiation and solvent-free conditions.[4,5] This powerful technique became extremely efficient and attractive in synthetic organic chemistry, and is able to activate many reactions due to cavitational collapse. Ultrasound irradiation provides higher yields and selectivities, shorter reaction times and milder reaction conditions, nontoxic, environmentally friendly solvent, in a one-step reaction, without isolation of any intermediate thus reducing time, saving money, energy and raw materials. In our research program focused for the synthesis of novel phosphonates derivatives with very timely methods. A series of new α-sulfamidophosphonateswere synthesized based on aliphatic linear sulfonamide containing nitrogen mustard moiety 1a,

various aromatic aldehydes 2a-2g and triethylphosphite by a one-pot three component condensation under ultrasonic irradiation at room temperature and solvent, catalyst-free conditions after 30 min-1 hours the reaction was completed with an excellent yields (Scheme 1).



Scheme 1 One-pot synthesis of α-sulfamidophosphonates containing nitrogen mustard moiety under ultrasound irradiation

Key words: Ultrasonic irradiation, Multicomponent reactions, solvent-free conditions, α-Sulfamidophosphonates.

Corresponding Email: m.guerfi@univ-alger.dz

References

[1] C. Hansch, PG. Sammes, Taylor JB (1990). In: Comprehensive Medicinal Chemistry, vol 2. Pergamon Press: Oxford, Chap.7.1

[2] M. H. Chen, Z. Chen, B. A. Song, P. S. Bhadury, S. Yang, X. J. Cai, D. Y. Hu, W. Xue, S. J. Zeng, Agric Food Chem, 2009, 57, 1383

[3] E. W. Petrillo (1980). US Patent 4,186,268, 1980, Chem Abstr, 1980, 93, 8008

[4] G. Gravotto and P. Cintas, Chem. Soc. Rev, 2006, 35, 180

[5] A. Amira, H. K'tir, M. Berredjem and N. E. Aouf, Monatsh. Chem, 2014, 145, 509.

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Effect of Gd3+ incorporation on structural and luminescence properties YAG phosphors powder doped with Ce3+ synthesized by sol-gel method

Sefiane Naima[a], Hamroun Mohammed Salah Eddine[b], Hadjou Belaid Zakia[c], Barka Wissem[d]

[a] Macromolecular Research Laboratory (LRM), Faculty of Sciences, Aboubekr Belkaid University,Tlemcen , Algeria
[b] Scientific and Technical Research Center in Physico-Chemical Analysis, Bp 384, Industrial Zone, Bou-Ismail CP 42004, Tipaza, Algeria
[c] Macromolecular Research Laboratory (LRM) , Faculty of Sciences , Aboubekr Belkaid University,Tlemcen , Algeria
[d] Macromolecular Research Laboratory (LRM), Faculty of Sciences, Aboubekr Belkaid University,Tlemcen , Algeria

Abstract:

In this paper, gadolinium yttrium aluminate ($(Gd_xY_{1-x})_3Al_5O_{12}:Ce^{3+}$) doped cerium phosphors with the different gadolinium concentration were achieved through synthesis via sol-gel method. The Gd^{3+} cationic substitutions in the YAG host matrix have been changed from 0 to 0.6 at%, and their effects on structural and photoluminescence properties were systematically investigated. The phosphors were characterized by X-ray diffraction (XRD), and photoluminescence (PL). Additionally, the evolution of crystallite size with the increasing of Gd^{3+} content is studied and discussed.

Key words: YAG: Ce; phosphors; photoluminescence; sol-gel.
Corresponding Email: naimasefiane1@gmail.com

References

[1] J. Amami, D. Hreniak, Y. Guyot, W. Zhao, G. Boulon, J. Lumin. 130 (2010) 603.

[2] Y.C. Wu, S. Parol, O. Marty, M. Villanueva-lbanez, J. Mugnier, Opt. Mater. 27(2005) 1471-1479.

ON-71

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Effect of temperature and pressure on the thermodynamic properties of $Fe_{2-x}NiGa_{1+x}$ Heusler alloys: An ab initio study

Sabah Chami [a], S. Lamari [a] and Z. Charifi [b]

[a] Department of Physics and Laboratoire d'Étude des Surfaces et Interfaces des Matériaux Solides, Faculty of Sciences, Ferhat Abbas University, Sétiif 1, Algeria
[b] Department of Physics, Msila University , Algeria

Abstract:

To gain a deeper understanding of the $Fe_{2-x}NiGa_{1+x}$ Heusler alloys, we carry out a systematic ab initio investigation of their thermodynamic properties using the Wien2k and Gibbs2 codes. The study revolves around the influence of temperature and pressure as more and more Fe atoms in the solid are substituted by Ga in this mixed phase. The following physical quantities are computed: The bulk modulus (B), specific heats at constant volume C_V and pressure C_P, Debye temperature θ_D, entropy S and thermal expansion coefficient α. We find that both the bulk modulus and Debye temperature increase with increasing pressure, however they exhibit a decreasing trend with temperature. In addition, it turns out that the specific heats C_V and C_P , the entropy and the thermal expansion coefficient are quite sensitive to both pressure and temperature.

Key words: Heusler alloys, thermodynamic properties,quasi-harmonic Debye model

Corresponding Email:

sachami_dz@yahoo.fr

References

[1]. M. A. Blanco, E. Francisco, and V. Luana, GIBBS: isothermal-isobaric thermodynamics of solids from energy curves using a quasi-harmonic Debye model, *Comput. Phys.*
[2] S.Chami et al. Eur. Phys. J. Plus (2021) 136:1147.

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Title: Study of the anti-corrosion properties of an expired drug for steel in hydrochloric acid: environmental protection.

D.ADDADJ[1.2], A. BERCHI[1], B. IDIR[2], M. DJAMA[2]

[1] Solid State Energy and Electrochemistry Laboratory, Department of Process Engineering, Faculty of Technology, U.F.A. Sétif 1, Sétif,19000, Algeria.

[2] Research Center in Industrial Technologies (CRTI), P.O.Box 64, Cheraga 16014, algiers, Algeria.

Abstract:

The use of corrosion inhibitors provides practical and economical solutions for many industrial sectors. This approach promotes resource conservation and reduces health and environmental risks. It underlines the growing importance of innovation in materials and engineering for sustainable and responsible industrial practices.

In this study, the use of an outdated drug as a corrosion inhibitor for steel in a corrosive medium of 1 M HCl was investigated. The inhibiting properties of the drug studied were examined over a range of concentrations at room temperature, using electrochemical methods as well as surface analysis techniques such as atomic force microscopy (AFM) and Fourier transform infrared spectroscopy (FTIR).

The results reveal that the expired drug has an inhibition efficiency of 93% at the optimum concentration. Through Potentiodynamic Polarization (PDP) analysis, it is observed that the drug examined acts as a mixed-type inhibitor, affecting both anodic and cathodic reactions. Electrochemical Impedance Spectroscopy (EIS) elucidates the inhibitor's ability to coat active sites on the metal surface, thereby reducing corrosion. In addition, surface analysis techniques (AFM and FTIR) confirm its significant role in preventing steel dissolution in acidic environments.
The study highlights the potential of expired drug as an effective corrosion inhibitor for steel in acidic environments.

Key words: Steel, Expired drug, Corrosion inhibitor, EIS, AFM, Environment.

Corresponding Email:

addadjdjouher@gmail.com

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

ÉVALUATION DE L'EFFICACITÉ DE L'HYDROXYDE DOUBLE LAMELLAIRE Mg-Fe POUR L'ÉLIMINATION DU BORE EN PESENCE DES IONS COMPÉTITEURS

Boukebbous Ines, et Boukhalfa-Djebbar Chahrazed

Laboratoire de pollution et traitement des eaux, Département de chimie, Université Frères Mentouri Constantine1, Algérie.

Résumé:

L'objectif de la présente étude est l'évaluation de l'efficacité d'un hydroxyde double lamellaire de magnésium et de fer (HDL Mg-Fe) dans l'élimination du bore dans l'eau en présence de différents ions. L'hydroxyde est synthétisé par la méthode de coprécipitation et caractérisé par différentes méthodes d'analyse texturale et structurale (DRX, ATR-FTIR, ATG-DTA, BET, pH_{PZC}). Les essais d'élimination du bore ont été réalisés en batch dans des solutions synthétiques et dans des eaux de distribution.

Les résultats obtenus, montrent que l'efficacité de l'HDL Mg-Fe synthétisé pour l'élimination du bore n'est significativement affectée par la présence des ions phosphate et des ions sulfate que pour des concentrations élevées de ces ions. Dans les solutions synthétiques ou dans les eaux de distribution, la cinétique d'élimination est rapide; le temps d'équilibre ne dépasse pas 30 minutes. Dans tous les cas, le taux maximal d'élimination est obtenu à pH: 9,5.

Mots clés: Bore, hydroxide double lamellaire, adsorption, traitement des eaux.

Corresponding Email : ines.boukebbous@doc.umc.edu.dz

ON-74

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Improved Mechanically Alloyed Fe-Mo-P Powders Properties for Industrial Exploitation

Sarra HARKATI[a,*], Wassila TEBIB[a], Saida BOUKEFFA[a] and Locif REDOUANI[a]

[a] Materials Physico-Chemistry Laboratory, Science and Technology Faculty, Chadli Bendjedid-Eltarf University, P.B. 73, Eltarf 36000, Algeria.

Abstract:

This study aims to produce Fe-Mo precipitates in the ternary Fe-Mo-P to enhance the strength of these alloys with high physical properties, such as heat and corrosion resistance as well as increasing hardness for many industrials applications (automotive, construction, oil, gas), with minimal damage to the environment and low coast. Thus, Fe-Mo-P samples were prepared using a high-energy ball milling process and characterized with X-ray diffraction. The data is processed through the Maud program which is based on the Rietveld method **[1, 2]**. Processing showed the formation of two phases the bcc α-Fe(P) solid solution and the tetragonal Fe-Mo binary precipitates with the average size reached after 7 hours of milling 53-118 nm, respectively, this was accompanied by a continuous decrease in the α-Fe(P) percentage in favour of the Fe-Mo. The solid state reaction pathway takes place via the dislocation, stacking fault and the antiphase bounderies.

Key words: Fe-Mo, Fe-Mo-P, XRD, Rietveld, SFP.

Corresponding Email: harkati-sarra@univ-eltarf.dz

References

[1] Lutterotti L. 2000 MAUD CSD Newletter (IUCR) No 24.

[2] Rietveld H. M. 1969 J. Appl. Cryst. 2 65.

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Half-metallicity from NaVAs half-Heusler alloy with stable structure in ferromagnetic state

Radja Nour El Imene Bennoui [a], Nawal Belmiloud [a], Fadila Belkharroubi[a]

[a] Laboratory of Analysis and Application of Radiations (LAAR), faculty of physics, University of Science and Technology of Oran Mohamed Boudiaf (USTO-MB) 1505 El Menouar 31000, Oran, Algeria.

Abstract

We investigate the structural, magnetic, and mechanical stability of NaVAs half-Heusler compound using the DFT based full-potential Wien2k package. Ferromagnetic, and non magnetic calculations are performed to ascertain the stable magnetic state. Calculations show that this compound is stable in the half-Heusler β-phase and the ferromagnetic state. The band structure and the density of states are obtained for GGA exchange correlation approximations. The electronic band structures and density of states reveal that NaVAs is a half-metallic ferromagnet (HMF). The calculated total magnetic moment of 3μB follows the Slater–Pauling rule. . Elastic constants were calculated to ascertain the mechanical stability of this compound.

Key words: NaVAs half-Heusler alloy, Ferromagnetic half-metal, Magnetic properties, First principles calculations.

ON-76

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Title: Préparation et caractérisation de matériau hybride à base de poly-2 Aminophényl disulfide renforcé par Silica Gel

S.BENYAKHOU[1*], A.BENYOUCEF[1]

[a] S.BENYAKHOU' Département de Génie des Procédés, Institut Des Sciences et Technologies, Université Mustapha Stambouli Mascara ,Algérie

[b] A.BENYOUCEF' Département de Génie des Procédés, Institut Des Sciences et Technologies, Université Mustapha Stambouli Mascara ,Algérie

Abstract:

Au cours des dernières années, les développements de matériaux hybrides inorganiques - organiques à l'échelle nanométrique ont reçu une attention particulière en raison d'une large gamme d'applications potentielles, le dopage d'oxydes inorganiques tels que TiO_2 [1-2], Silica [3, 4], MoS [5], Fe_3O_4, ZnO, Al_2O_3 [8]. Ces hybrides polymères / inorganiques présentent de nombreux nouveaux caractères, tels que les propriétés électriques, optiques, catalytiques et mécaniques que le matériau unique n'a pas.

Le matériau du gel de silice a attiré beaucoup d'attention au cours des dernières décennies en raison de ses propriétés uniques, telles qu'une excellente réactivité magnétique, une distribution uniforme de la taille des pores, une surface élevée, une faible cytotoxicité, etc. Pour cela, SiO_2 est un choix préférentiel pour séparer toutes les nanoparticules polymères du contact direct. Bien que la polymérisation de l'aniline et leur dérivé sur la surface de SiO_2 a été facilement réalisé pour obtenir le polymère / SiO_2. En outre, le revêtement total de SiO_2 sur polymère a limité l'application des noyaux car le matériau cible de chargement n'a pas d'espace effectif pour interagir avec le polymère.

Dans ce travail, nous étudions l'effet des additifs différentes quantités de nanoparticules de SiO_2 (0,5g, 1.5g et 2g) sur les propriétés des composites synthétisés chimiquement par oxydation in situ en utilisant du monomère disulfure de 2-aminophényle, de l'acide chlorhydrique comme dopant et persulfate d'ammonium comme oxydant. Les propriétés des nanocomposites ont été étudiées et comparées à celles du poly (2APhS) pur. Ils ont été caractérisés en utilisant différentes techniques: FTIR, UV, XRD et TGA. Les résultats confirment la formation réussie des composites. La morphologie de surface des échantillons a été caractérisée par microscopie électronique à transmission (TEM). Les images obtenues montrent la formation de poly (2APhS) sur la surface De renfort. Les échantillons résultants gardent toujours des conductivités élevées.les conductivités électriques ont été mesurées en utilisant la méthode de sonde à quatre points. Le comportement électrochimique du poly (2APhS) séparé du SiO_2 a été analysé par voltamètre cyclique.

Key words: Poly2 Aminophényldisulfide ; Polymères conducteurs ; nanocomposites ; dioxyde de silice ; propriétés électrochimique.

Corresponding Email:

samihasamiha51@yahoo.fr

References

[1] F. Chouli, I. Radja, E. Morallon, A. Benyoucef. A Novel Conducting Nanocomposite Obtained by p-Anisidine and Aniline With Titanium(IV) Oxide Nanoparticles: Synthesis, Characterization, and Electrochemical Properties. Polymer Composites. DOI 10.1002/pc.23837.

[2] L. Shi, X. Wang, L. Lu, X. Yang, X. Wu, Preparation of TiO2/polyaniline nanocomposite from a lyotropic liquid crystalline solution, Synthetic Metals 159 (2009) 2525-2529.

[3] Katarzyna Depa, Adam Strachota, Miroslav Šlouf, Jiří Brus, Věra Cimrová. Synthesis of conductive doubly filled poly(N-isopropylacrylamide)-polyaniline-SiO2 hydrogels. Sensors and Actuators B: Chemical. 244 (2017) 616-634.

[4] Ying Dan Liu, Fei Fei Fang, Hyoung Jin Choi, Yongsok Seo. Fabrication of semiconducting polyaniline/nano-silica nanocomposite particles and their enhanced electrorheological and dielectric characteristics. Colloids and Surfaces A: Physicochemical and Engineering Aspects. 381 (2011) 17-22.

[5] Gang Fu, Li Ma, Mengyu Gan, Xiuling Zhang, Meng Jin, Yao Lei, Peishu Yang, Maofa Yan. Fabrication of 3D Spongia-shaped polyaniline/MoS2 nanospheres

ON-77

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Ab-initio Study of Structural, Electronic And Optical Properties Of $AgAlTe_2$ Compound in the framework of DFT

Louati Nesrine[a], Boudjaadar Djamel[b], Ouarda nemiri[a], Faycal Oumelaz[a], Gouasmia Wissem[a], Sonia Chebouki[a]

[a] Department of physics, Institute, Higher Normal School of Technological Education of Skikda, Algeria
[b] Department of physics, Institute, LRPCSI-University of auguest 20th 1955 Skikda, Algeria

Abstract:

In recent years, I–III–VI_2 chalcopyrite compounds have attracted considerable attention due to their properties.These types of semiconductor materials have thrilled structural, electronic, optical, …, and termal properties , resulting in many applications such as in : photoelectrochemical (PEC) systems, optoelectronic and nonlinear optical devices including solar cells.Motivated by these properties, we conducted a study on $AgAlTe_2$.

In this work, we presented an ab-initio study of the structural, electronic and optical properties of AgAlTe2 ,Our calculations were congucted using augmented plane wave (FP-LAPW), based on the density functional theory (DFT) and implemented in the calculation code Wien2k.The results of our calculation of the lattice constants are a=b=6.2683°A, c=12.2396°A .The energy gap is about 2.0459 eV which are well agree with experimental data and the previous theoretical study .The optical properties of the titled compound which are described by the dielectric function are calculated .

Key words: chalcopyrite, semiconductor, DFT, FP-LAPW

Corresponding Email:

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Elaboration and Characterization of Copper-doped tin Oxide Thin films for Photovoltaic applications

BarkatLamia, Benameur Khedidja
Universityof Oran 1 Ahmed Ben Bella (Oran)

Abstract

In this study , we present the results of morphological, structural and optical analysis of Cu-doped SnO2 thin films elaborated by dipcoating . The effects of Cu doping on the morphological , structural and optical properties of SnO2 thin films werein vestigated by atomic forcemicroscopy (AFM), X-raydiffraction (XRD) and UV-Visspectroscopy. XRD diagrams of Cu-doped SnO2 films show that the films are crystallized in the face-centered cubic phase , and that the crystallinity of SnO2 films degrades with increasing Cu content. AFM images showed the formation of agglomerateson the surface of Sn1-xCuxO films. The optical characteristics of the samples show that Sn1-xCuxO thin films are transparent in the visible range.

ON-79

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Title: **DFT Calculation of the Structural, electronic and optical properties of the chalcopyrite compound $MgSiP_2$**

O. Drici, H.Meradji, S. Ghemid

[a] ***Physics Department, Badji Mokhtar-Annaba University, Algeria***

[b] ***Physics Department, Badji Mokhtar-Annaba University, Algeria***

[c] ***Physics Department, Badji Mokhtar-Annaba University, Algeria***

Abstract:

In this work, we studied the structural, electronic and optical properties of the chalcopyrite compound MgSiP2 using the Linearized Augmented Planar Wave (LAPW) method implemented in the framework of density functional theory (DFT) by employing the Wien2k computational code. The generalized gradient approximation (GGA) for the exchange and correlation potential (XC) term was used to study the structural properties.

The variation of the lattice parameter, compressibility modulus and energy gap of MgSiP2 compound as a function of the composition show a non-linear dependence. For the optical properties we made qualitative studies for some optical constants, such as dielectric function, refractive index, and reflectivity, which were evaluated in the energy range (0-30) eV, performed at the level of mBJ exchange potential, the obtained results agreement with the experimental data.

Key words: FP-LAPW, GGA, Chalcopyrite, DFT, Wien2k

.....

Corresponding Email: Oussama.drici@univ-annaba.dz

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Influence of Charge Transfers on two-Photon absorption cooperative effects within multi-Dipolar Ruthenium Complexes

Anissa Amar[a], Abdou Boucekkine[b], Nicolas Durand, Huriye Akdas-Kiliç[b] , Jean-Luc Fillaut[b]

[a] Laboratoire de Physique et Chimie Quantiques, Faculté des Sciences, Université Mouloud Mammeri de Tizi-Ouzou, Tizi-Ouzou 15000, Algeria.
[b] Univ. Rennes, CNRS, ISCR (Institut des Sciences Chimiques de Rennes) UMR 6226, 35000 Rennes, France.

Abstract:

One and two-photon characterizations of a series of hetero- and homoleptic [RuL3-n(bpy)n] 2+ (n = 0, 1, 2) complexes carrying bipyridine π-extended ligands (L), have been carried out. These π-extended D−π−A−A−π−D-type ligands (L), where the electron donor units (D) are based on diphenylamine, carbazolyl, or fluorenyl units, have been designed to modulate the conjugation extension and the donating effect. Density functional theory calculations were performed in order to rationalize the observed spectra. Our calculations show that the electronic structure of the π-extended ligands has a pronounced effect on the composition of HOMO and LUMO and on the metallic contribution to frontier MOs, resulting in strikingly different nonlinear properties. This work demonstrates that ILCT transitions are the keystone of one- and two-photon absorption bands in the studied systems and reveals how much MLCT and LLCT charge transfers play a decisive role on the two photon properties of both hetero- and homoleptic ruthenium complexes through cooperative or suppressive effects.

Key words: DFT, two-Photon absorption, Charge transfer, Ruthenium Complexes

Corresponding Email:
Anissa.amar@ummto.dz

ON-81

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Adsorption of methylene blue dye from a liquid solution using an organometallic material based on iron nitrate

AFOUN Meryem*, BENNABI Souad, HEDIDI Madani

Department of Chemistry, Faculty of Exact Sciences and Informatics, University of Hassiba Benbouali, B.P 78C, Ouled Fares, Chlef, Algeria

Abstract:

Adsorption is a widely used technology for the separation and removal of dyes from wastewater. However, the dye removal process using conventional adsorbents is not sufficiently efficient for industrial wastewater [1]. Metal-organic frameworks (MOFs) addresses these drawbacks. MOF showed excellent dye removal and degradation capacity owing to its multifunctionality, water-stability, large surface area, tunable pore size and recyclability [2]. In this perspective, we decide to prepare a new MOF based on Iron(III) nitrate nonahydrate for the metal part and pyromellitic acid as organic ligand by solvothermal method using DMF as solvent. Then, we tested the efficiency of this material for the adsorption of the methylene blue dye from aqueous solution and the obtained results showed that the maximum adsorption uptake is 20,833 mg/g.

Key words: MOF, adsorption capacity, Methylene Bleu dye, water treatment.

Corresponding Email: m.afoun@univ-chlef.dz

References

[1] Bao J., Li H., Xu Y., Chen S., Wang Z., Jiang C., Li H., Wei Z., Sun S., Zhao W., J. Mater. Sci. Technol., 78, 131–143, 2021.

[2] Furukawa H., Cordova K E., O'Keeffe M,. Yaghi M O., Science, 341, 2013.

Application of Heusler Materials in the Reduction of Greenhouse Gas Emissions

Hamadi Zineb 1 , Bendahma Fatima 1 , Bessaha Fatiha 2 ,

1 Laboratory of Technology and Solid Properties, Abdelhamid Ibn Badis University, Mostaganem, Algeria

2 Structure Development and Applications of Molecular Materials, Abdelhamid Ibn Badis University, Mostaganem, Algeria

Abstract:

Energy plays an important role in the development of countries. Currently, thermoelectric materials such as Heuslers alloys directly convert residual thermal energy into useful electrical energy. These materials could play a crucial role in the prevention of the energy crisis, as well as in the reduction of greenhouse gas emissions, ie by serving as a source of green energy. In this context, our work consists of studying the thermoelectric performance of a Heusler material, namely KCaC. The semi-classical theory of Boltzmann implemented in the BoltzTraP code is applied to study the thermoelectric properties (TE). The high value of the figure of merit (ZT = 0.98) was achieved to make the KCaC compound a promising candidate for TE applications.

Key words: Heusler material, Greenhouse effect, Energy crisis.

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Electronic and optical properties of strained Al1-xGaxN

Rim roukya Belhoula, Azzedine Telia ; Abdelhakim Meziani

Abstract

Nitrides like AlGaN and AlInN and InGaN and their hetrostructures are usually epitaxially grown on a foreign substrate, such as sapphire [1]. Due to the large differences in lattice parameters and thermal expansion coefficients between the substrate and the nitride over-layers, and between nitride layers with different alloy compositions, strain is always present in group-III nitride based devices influencing the physical properties [2]. Based on this, we present a study of the variation of the structural, electronic and optical properties of "AlGaN" with tensile and compressive strains. For an improved description of the above cited properties we use Density Functional Theory (DFT) , as implemented in the Quantum Espresso Package [3]. The structural properties were treated using PBE [4] exchange-correlation energies while the band gap was calculated using the modified Becke-Johnson (MBJ) potential [5].

References :

[1]A. Minj, D. Cavalcoli, A. Cavallini n.2011 Elsevier .

[2] D.Cavalcoli, A. Minj, S Pandey and A. Cavallini, International Conference on Defects in Semiconductors 2013 AIP Conf. Proc. 1583, 301-304 (2014); doi: 10.1063/1.4865657

[3]P Giannozzi et al, Journal of Physics: Condensed Matter, Volume 29, Number 46,2017

[4] J.P. Perdew, Y. Wang, Phys. Rev. B 45 (1992) 13244.

[5] F. Tran, P. Blaha, Phys. Rev. Lett. 102, (2009) 226401.

ON-84

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Title: Removal of Heavy Metals from Wastewater by Coal.

Sadaoui Loubna[a], Djebabra Sihem[b], Rahali Hanane[b], Bekiri Fadia[c], Hamdi Ines[b], Bouzid Khadidja[c], Charif Majda[a].

a' Laboratory of LARGHYDE, University of Biskra Bp 145 RP, Biskra 07000, Algeria.
b' Industrial chemistry Department, University of Biskra (07000), Algeria.
c' Scientific and Technical Center Research on Arid Regions, University of Biskra (07000), Algeria.

Abstract:

Industrial activities play a significant role in the emission of environmentally harmful substances, particularly heavy metal ions, which pose a threat to various organisms, including humans. The primary aim of this research is to eliminate heavy metals from industrial wastewater through the process of adsorption, utilizing activated carbon derived from a naturally occurring biomass waste. The utilization of this commonly found environmental concern as the fundamental material for biochar formation is a key aspect of this study.The Biochar was thoroughly characterized using GTA and Infrared spectroscopy analyses FTIR. The adsorption experiments were conducted under different conditions: solution pH zero, contact time.

Key words: biochar, heavy metals, removal, wastewater.

Corresponding Email:

loubna.sadaoui@univ-biskra.dz

ON-85

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

The Impact of Exterior Walls on Algerian Rural Buildings' Energy Efficiency in Various Climate Zones

Horiya Benharchache[a], Fouad Khaldi[b], Morad hanfer[c], …

[a] Laboratory of Physics and Applied Energy (LPEA), University Batna-1-, Batna 05000, Algeria
[b] Higher National School of Renewable Energy, Environment & Sustainable Development, Batna 05000, Algeria
[c] Faculty of Natural Sciences, University of Batna 2,Constantine way 53, Fesdis, Batna 05078,Algeria

Abstract:

One of the biggest users of resources is the construction industry (energy and materials). This source provides about 42% of Algeria's primary energy, and it is expected that this number will increase as the nation's population increases, particularly in rural areas where urban expansion is occurring. This study's objectives are to assess the orientation of rural buildings, glazing systems, and the viability of utilizing two distinct kinds of rural constructions. The first type of wall, known as ordinary walls (W1), is the most often used type. The second type of HEP (W1, W2) is dependent upon thermal insulation; Polysterene represents the first type, while the second type is a locally accessible bio-composite date palm fiber. Three primary dominating climates in Algeria were used for this investigation. Various numerical experiments were conducted using the EnergyPlus software in order to achieve this goal. The findings demonstrated how the building's orientation was impacted by various climate zones. The optimal orientation for rural buildings is south, north, and east for Algiers, Batna, and Tamanrasset, respectively. In Tamanrasset, small windows with a 20% window-to-wall ratio contribute to energy savings of 27.3% and 18.3%. Conversely, in Batna, a window-to-wall ratio of 30% to 40% is ideal for medium-sized windows. The outcomes demonstrate the efficacy of the wall W3, which incorporates bio-composite DPF, in lowering the yearly total thermal energy by roughly 45%, 20%, and 5%, respectively, in the three climates of Algiers, Batna, and Tamanrasset.

ON-86

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Title: A Comprehensive Analysis and Identification of Lemaitre damage model parameter of DC04 metal sheet

Presenting author's : MECHENENE Mohamed lamine[a], ZAAF Mohamed[b], CHAHAOUI Oualid[c] MATOUGUI Nedjoua[a]

[a] L3M Mining, Metallurgy and Materials Laboratory, *National Higher School of Technology and Engineering (ENSTI Ex ENSMM)*, Annaba, Algeria.
[b] Metallic Materials Forming Laboratory (LMF2M), *Badji Mokhtar University UBMA*, Annaba, Algeria.
[c] I.S.M.A Laboratory, *Laghrour-Abbes University*, Khenchela, Algeria.

Abstract:

The objective of this work is to analyze the elastoplastic damage behavior of DC04 via the Lemaitre model. The experimental part is carried out by carrying out loading unloading and monotonic traction tests. The damage parameters are obtained via a mechanical behavior function from experimental data and compared to a numerical simulation.

It was concluded that the Lemaitre damage model could be successfully applied to the DC04 sheet, in order to predict it is initiation of damage during material forming as well as to understand its progression until failure.

Key words: Lemaitre ductile damage Model, load-unloading tensile tests, Metal-Forming process, Numerical Simulations, DC04 metal sheet.

Corresponding Email: m.mechenene@etu.ensti-annaba.dz

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Title: Doped Bio-Calcium with semi-conductor (Aurivillius) for the Degradation and elimination of organic polluants

Charif Majda[a], Rehali hanane[b], Menasra hayet[c], Ben brika chaima[c], Saadaoui lobna[a], Rais zineb[a]

[a] Laboratory of LARGHYDE, University of Biskra Bp 145 RP, Biskra 07000, Algeria

[b] Industrial chemistry Department, University of Biskra (07000), Algeria

[c] applied chemistry laboratory, material science faculty, University of Biskra (07000), Algeria

Abstract:

This study examines the conversion of waste biomass into biochar, using a unique procedure that involves the insertion of a ceramic material. The use of biomass waste, which is a significant environmental issue, served as the primary material for the production of biochar. Additionally, the ceramic was added to improve the structural and functional characteristics of the biochar. The composite material was thoroughly characterized using Diffraction X-ray (DRX), scanning electron microscopy (SEM) and Infrared (FTIR) spectroscopic investigations.

The combination of waste biomass-derived biochar with the inserted ceramic material demonstrates the potential benefits of this new biocomposite. Its enhanced structural stability and altered functional groups underscore its potential for diverse applications, ranging from environmental remediation to industrial utilization.

This work introduces a new method to make use of waste biomass and emphasizes the importance of adding ceramic materials to improve the qualities of the resulting biochar. This opens up possibilities for using biochar in a sustainable and diverse way.

Polymeric Nanocapsules Loaded with 5-Fluorouracil for Targeted Cancer Therapy

Kheira ZANOUNE [1] , *Mohammed DELLALI* [1] , *Delia Mihaela Rata* [2], *Marcel POPA* [3,4]

[1] *Faculty of Technology , Hassiba Benbouali University of Chlef, Algeria, zanounekheira@yahoo.fr;*
[2]*Faculty of Medical Dentistry, Apollonia University of Iasi, Romania*
[3] *"Gheorghe Asachi" Technical University of Iasi, Romania,*
[4]*Academy of Romanian Scientists, Bucuresti, Romania*

ABSTRACT

Cancer remains one of the world's most devastating diseases, and the number of new cases increases each year [1]. Conventional delivery of chemotherapeutic agents led to the fast development of cellular resistance causing toxic side effects (cytotoxicity, neurotoxicity, nephrotoxicity) on the entire body which limits the drug doses that can be administrated [2]. Drug delivery systems can play a key role in the fight against cancers by delivering locally, to the tumor site, the anticancer drugs. The efficiency of this delivery depends on several factors, such as: drug bioavailability, drug absorption processes, pharmacokinetic processes, timing for optimal drug delivery [3]. The use of drug-loaded nanocapsules offers great opportunities for the development of new non-invasive strategies for the treatment of cancers, due to their capacity to accumulate in tumors by enhanced permeability and retention effect [4.5]. The main purpose of this study was to obtain polymeric magnetic nanocapsules, based on chitosan, poly(N-vinylpyrrolidone-*alt*-itaconic anhydride) copolymer, and maghemite as colloidal magnetic nanoparticles, in order to deliver the model drug (5-Fluorouracil – 5-FU) to the cancer cell in a targeted and sustained way. The interfacial condensation process used for the preparation of nanocapsules does not require any kind of crosslinking agents, often toxic and difficult to remove from the synthesis products. The condensation reaction took place at the interface between the two solutions by opening the anhydride cycles from the copolymer, under the action of the NH_2 groups from chitosan. FTIR spectroscopy revealed the formation of amide bonds in the membrane of these nanocapsules. SEM provided more information on the shape and size of nanocapsules. The magnetic properties of the magnetic material and magnetic polymeric nanoparticles were obtained by vibrating sample magnetometer at room temperature. Synthesized nanocapsules showed spherical shape and their diameter varies between 100–200 nm as a function of the molar ratio of the polymers. All analyzed samples showed a rapid swelling due to the penetration of water inside the capsule and into/through the polymer membrane, followed by a slower swelling to equilibrium. 5-Fluorouracil (5-FU) loading and release capacity was studied, the processes being controlled by the drug diffusion through the polymeric membrane. The obtained nanocapsules are biocompatible, which is confirmed by their lack of toxicity (cell viability is high in their presence) and hemocompatible. At this time, our results indicate that polymeric magnetic nanocapsules can have a great potential as a new type of drug delivery system for tumor treatment. In order to demonstrate the targeting effect of the aptamer functionalized nanocapsules, additional in vitro studies are carried out at the present.

Keywords : Synthesis , Nanoparticles, natural and synthetic polymers , drug delivery systems , 5-Fluorouracil.

REFERENCES:

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Optimizing Performance of $KSnI_3$-Based Perovskite Solar Cells with Tin (Sn) using SCAPS Software

Badiaa BACHIRI[a,b], Khadidja RAHMOUN[a,b]

[a]*Department of physics, Faculty of sciences, University of Tlemcen AbouBekr Belkaid, Tlemcen Algeria*
[b]*Unit of Research on Materials and Renewable Energies, URMER, Tlemcen, Algeria*

Abstract:

This research paper studies perovskite solar cells using tin (Sn) as the base material and employing SCAPS software for analysis, focusing on the absorbing KSnI3 perovskite layer[1]. The study reveals key results including fill factor (FF) of 88.27%, power conversion efficiency (PCE) of 15.51%, open circuit voltage (Voc) of 1.2871 V and a short-circuit current density (Jsc). of 13.653229 mA/cm². Furthermore, the investigation identifies that the optimal thickness of the KSnI3 layer is 1 µm, resulting in a remarkable PCE of 19.4257%. The research also highlights the impact of defect density on performance, showing that an increase in the number of defect sites leads to more traps and recombinations paths, ultimately reducing efficiency. These results highlight the potential of KSnI3 [2]-based perovskite solar cells as viable candidates for high-efficiency photovoltaic applications.

Key words: Perovskite solar cells, $KSnI_3$, Power conversion efficiency, SCAPS 1D

Corresponding Email: bachiribadi3a@gmail.com

References

[1] G. Pindolia, S. M. Shinde, and P. K. Jha, 'Non-leaded, KSnI3 based perovskite solar cell: A DFT study along with SCAPS simulation', *Materials Chemistry and Physics*, vol. 297, p. 127426, Mar. 2023, doi: 10.1016/j.matchemphys.2023.127426.

[2] B. Bachiri and K. Rahmoun, 'Numerical Simulation of Perovskite Solar cell with Porous Silicon layer', p. 6, 2022.

ab initio study of the structural and electronic and Optical properties of The New Double Perovskite

Chikh Ali.HADJI [1,2,*], Amina. ARRAR[1,2], Mohamed.GHALEB [1,2], zaza TOUAA [1,2]

[1] Department of Physics, *Faculty of Technology*, *University of RELIZANE, BOURMADIA, BP 48000, W. Relizane, Algeria.*

[2] *Laboratory of Physics Thin Layer & Advanced Technologies*, *University of RELIZANE, Bourmadia, BP 48000, W. Relizane, Algeria*

. chikhali.hadji@univ-relizane.dz

Abstract:

In this work, we report the structural and electronic properties of new double perovskite , these properties are investigated with the first-principles methods based on density functional theory (DFT) [1,2] using the Generalized Gradient Approximation (GGA) [3, 4] for the exchange correlation functional. In this approach, we used the Full Potential Linearized Augmented Planes waves (FP-LAPW) [5] methods as embedded in Wien2k code [5]. The optimized lattice parameters are obtained as 14.3 Å for the material in face-centered cubic structure ($Fm\bar{3}m$ space group). The first-principles calculations have given the energy gaps values as 2.658 eV.

***Keywords*:** electronic properties, Solar cell, Density functional theory, Double-perovskite, Lead-free, WIEN2k code, FP-LAPW+ DFT

Refence

[1].P. Hohenberg and W. Kohn. Phys. Rev., 136:B864(1964).
[2].Perdew J P, Chevary J A, Vosko S H, Jackson K A, Pederson M R, Singh D J and Fiolhais C 1992Phys. Rev.B 466671(1992).
[3].Perdew, JP, Burke, K, Ernzerhof, M: Generalized gradient approximation made simple. Phys. Rev. Lett.77, 3865 (1996).
[4].Perdew J P and Wang Y 1992Phys. Rev.B4513 244(1992).

ON-91

ICMSE'2024

The 3rd edition of the international conference on materials science and engineering and their impact on the environment

Title: Electrochemical characterization of the AMX anion exchange membrane in buffered solution.

Abdallah Timmaoui[a], Mahmoud Ferhat[a]

[a] Matter sciences Department, Faculty of sciences, University of Laghouat, Algeria.

Abstract:

Membrane technology has gained increasing significance in industrial separation processes, desalination, and wastewater treatment. It plays pivotal roles in various industries such as food processing, pharmaceuticals, and petrochemicals. Over the past two decades, membrane technology has been increasingly utilized to tackle water scarcity through wastewater reclamation and desalination. Electrodialysis (ED) stands out as one of the most prevalent membrane separation processes, driven by an electric field gradient enabling the separation of minerals from feedwater solutions. It generates two distinct streams - a desalinated flow termed diluate and a concentrated flow termed concentrate. However, operational challenges in electrodialysis may arise, including inorganic salt precipitation on membrane surfaces, membrane degradation, and elevated energy consumption due to concentration polarization at the membrane-solution interface during mass transport. A comprehensive understanding of concentration polarization is crucial for enhancing membrane performance, process efficiency, and reducing operational costs. In this study, we enhanced mass transport through the membrane by introducing an ammonia buffer. Results demonstrate that ammonia addition facilitates counter-ion transfer, completely eliminating system polarization, and catalytically enhancing the water dissociation reaction in the boundary layer. This shift towards ohmic regions by destruction and elimination of the diffusion boundary layer improves overall process efficiency.

ON-92

ICMSE'2024

The 3rd Edition of the International Conference on Materials Science and Engineering and Their Impact on the Environment

The influence of nanoparticles on the behavior of droplet generation.

Bourega Mohammed[a], Soulimane Soufiane[b]

[a] Biomedical Engineering Laboratory, Biomedical Engineering Department, University Abu Bakr Belkaid, Tlemcen, Algeria.
[b] Biomedical Engineering Department, University Abu Bakr Belkaid, Tlemcen, Algeria.

Abstract:

In this work, we focus on the digital microfluidics [1] domain which uses the manipulation of micro-and nano-droplets from two non-homogeneous fluids such as water and oil. Our research is based on the use of the T-junction [2], [3] (A straight channel receives the continuous phase and a lateral channel where the dispersed phase flows) to study the passive control of the size and generation rate of micro/nano-droplets. For that, we use the finite element method by using the ANSYS Fluent to establish a parametric analysis. A lot of studies have been widely used in the areas of nanomaterials preparation, pharmaceutical analysis, and protein engineering[1], [4]. In this study, we are interested in droplet formation in the presence of nanoparticles. We studied the influence of the fluid's velocity ratio and its impact on the size and the generation rate of the micro/nanodroplets. Where the water is mixed with nanoparticles as inlet fluid in the continuous phase of the T junction, and oil is used as the dispersed phase. Thus, the ratio ($\upsilon = \upsilon_w / \upsilon_o$) is defined as water velocity (υ_w) to oil velocity (υ_o). The results show that when the ratio (υ) increases the length of the droplet decreases (from 90 µm to 14 µm) and the generation rate increases. Moreover, as the concentration of nanoparticles increases and the velocity ratio is fixed at $\upsilon = 20$, the droplet length decreases and the generation rate increases.

Keywords: Digital Microfluidic, droplet formation, nanoparticles, T-shaped microfluidic, numerical simulation, fluid dynamics.

Corresponding Email: mohammed.bourega@univ-tlemcen.dz

References

[1] S. D. Ling, Z. Liu, W. Ma, Z. Chen, Y. Du, and J. Xu, "A Novel Step-T-Junction Microchannel for the Cell Encapsulation in Monodisperse Alginate-Gelatin Microspheres of Varying Mechanical Properties at High Throughput," *Biosensors*, vol. 12, no. 8, p. 659, Aug. 2022, doi: 10.3390/bios12080659.

ON-93

Synthesis and characterization of Ce_xMn_Y-Mg_4Al_2 hydrothalcite based system. Application in catalytic oxidation of n-butanol

N. Haddad[a], F. Sahraoui[a] and J.F Lamonier[b]

[a1]Laboratory of Chemistry of Natural Gas, Faculty of Chemistry (USTHB), BP 32, 16111, Algiers, Algeria

[b] Univ Lille Nord de France, USTL, Unité de Catalyse et de Chimie du Solide, UMR CNRS 8181, 59652 Villeneuve d'Ascq, France

Abstract:

Industrial processes release a plethora of volatile organic compounds (VOCs) into the atmosphere, which adversely affect human health. To tackle this issue, catalytic oxidation has emerged as a promising solution for the complete elimination of VOCs [1]. In this context, our study investigates Ce and Mn-containing MgAl LDH, focusing on its structural and catalytic properties. The Mn_XCe_Y-Mg_4Al_2-HT systems (with x = 0, 0.4, 0.6, and 0.8, and x+y=0.8) were prepared using a two-step calcination-reconstruction process. The effects of cerium and manganese content on the structural and catalytic properties of Ce and Mn-containing MgAl LDH were investigated. The samples underwent characterization using XRD, BET, Raman, XPS, and ATG techniques. The catalytic activity of the resulting compound in n-butanol oxidation was examined.

Increasing Ce and/or Mn contents led to changes in the structural, textural, and reducibility properties of the synthesized systems. The catalyst with high Ce content (x= 0.8 and 0.4) exhibited the highest catalytic activity, particularly for x = 0.8. Conversely, the addition of a low amount of Mn to the system ($Ce_{0.6}Mn_{0.2}$-Mg_4Al_2) significantly improved CO_2 formation. The formation of active sites occupied by cerium and manganese within the LDH structure, contributed to the material's performance. The Ce^{3+}/Ce^{4+} and Mn^{3+}/Mn^{4+} redox couples in the external layers enhanced O_2^- diffusion and their activation into nucleophilic species, facilitating butanol transformation.

Key words: Catalytic oxidation; n-Butanol; Hydrotalcite; Cerium, Manganese

Corresponding Email: Akrour_naima@hotmail.com

References

[1] Górecka, S.; Pacultová, K.; Fridrichová, D.; Górecki, K.; Bílková, T.; Žebrák, R.; Obalová, L. *Materials* 2021, *14*(21), 6581.