

Humboldt-Kolleg / International Conference Organized by

Djillali Liabes University of Sidi Bel-Abbes:

*Laboratoire de Microscopie, Micro-analyse et Spectroscopie Moléculaire & Laboratoire
des Matériaux Magnétiques*

with the cooperation of

The University Aboubar Belkaid of Tlemcen:

Unité de Recherche Matériaux et Energies Renouvelables

Theory and Computation in Sciences and Bio-Sciences
TCSBS 2014

November, 15 - 18, 2014

Tlemcen - Algeria



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Invited speakers

Prof. Dr. Michael Springborg (Germany): Response of large systems to static electromagnetic fields

Prof. Dr. Reinhold Fink (Germany): Applying Computational Chemistry on Material Properties in Organic Electronic Devices

Prof. Yoon Sup Lee (Korea): Protocols to calculate redox potentials of transition metal complex ions

Prof. Dr. Henning Hopf (Germany): Aromatic Chemistry 150 Years after Kekulé: From the Plane to Three-dimensional Space

Prof. Dr. Karin Fink (Germany): Transition metal compounds in magnetism and catalysis

Prof. Dr. Lotfi Belkhiri (Algeria): Relativistic computational study of highly selective N-ligands for Ln(III)/An(III) separation

Prof. Dr. Gérard Vergoten (France): A cybernetic approach to molecules, molecular recognition and chemical communication

Dr. Aurélien Moncomble (France): Elucidation of metal complex structures by time dependent DFT calculation coupled with electronic spectroscopies

Prof. Dr. Dalila Hammoutène (Algeria): Computational Molecular Design of Optimal Nonlinear Optical Materials

Dr. Sahar Abdalla (Soudan): Isolated and deposited potassium clusters

Prof. Dr. Marwan Mousa (Jordan): Microwave Harmonics Generated in Laser-Assisted Scanning Tunneling Microscopy- Their Significance Regarding Terahertz Sources in Laser Assisted Field Emission

Prof. Dr. Aziz Aboulmouhajir (Morocco): Molecular modeling petro chemistry and therapeutic chemistry

Prof. Dr. Lounis Mourad (Algeria): Crash energy dissipation in the head security helmet

Prof. Dr. Mohamed Ellouze (Tunisia): Critical behavior in Fe-doped manganites



$\text{La}_{0.67}\text{Ba}_{0.22}\text{Sr}_{0.11}\text{Mn}_{1-x}\text{Fe}_x\text{O}_3$ ($0 < x < 0.2$)

Prof. Dr. Hans-Heinrich Limbach (Germany): NMR Studies of acid-base interactions: from hydrogen bonded model systems to proteins

Prof. Dr. Hossein Eslami (Iran): Molecular Dynamics Simulation of a Polyamide-Nanotube Nanocomposite

Prof. Dr. Mohamad Elkhateeb (Jordan): Organoiron selenocarboxylate Complexes: Synthesis, characterization and Reactivity

Prof. Dr. Cenk Selcuki (Turkey): Molecular Modeling of Metal ion interactions with Biochemical Molecules

Dr. Alberto Del Rio (Italy): Computational design of bioactive compounds: past, present and future

Prof. Dr. Abdelkader Souifi (France):

Prof. Dr. Ashraf Abadi (Egypt): Mining ZINC Database to Discover Potential Phosphodiesterase 9 Inhibitors Using Structure-Based Drug Design Approach Industry

Prof. Dr. Saber Chatti (France): Synthesis and characterization of polymers from biosourced monomers.

Prof. Dr. S. Mohamed Mekelleche (Algeria): Theoretical study of the mechanism, regio- and stereo-selectivity of cycloaddition reactions.

Dr. Sayede Adlane (France): Insight on the ferroelectric properties in $(\text{BiFeO}_3)_2(\text{SrTiO}_3)_4$ superlattice: from experiment and ab initio calculations

Dr. Sami Lakhdar (France): Phosphido-Boranes: Old Molecules with New Insights

Prof. Dr. Yasseen Alsoud (Jordan): Synthesis and Biological Evaluation of Phenyl Substituted 1H-1,2,4-Triazoles as Non-Steroidal Inhibitors

Dr. Fawzi Lakrad (Morocco): Nonlinear vibrations in Atomic Force Microscopy systems

Dr. Ahmad Telfah (Germany): Online Nuclear Magnetic Resonance (NMR) detection of mass and volume limited living cancer cell and other biological samples

Dr. Samir El Zein (Liban): stock markets simulations: from maths to clients

Dr. Ismail Trabelsi (Tunisia): Co-pyrolysis of landfill leachate reverses osmosis concentrate with sewage sludge in a fixed-bed reactor

Prof. Dr. Nasser Chellouah (Algeria): Calcined clay in the futur cement.

Prof. Dr Mostefa Belkhatir (Algeria): Laboratory Study on Static Liquefaction of Overconsolidated Silty Sand Soils: Effect of Sample Preparation

Prof. Dr Latifa Debbi (Algeria): How the study of the fractional Navier-Stokes equation helps in the understanding of the millennium problem

Prof. Mohamed Hedi Ben Ghazlen (Tunisia): Influences of anisotropy on band gaps of 2D photonic crystal with hexagonal inclusions

Prof. Dr A. Maalej (Tunisia): *Performance evaluation of an agro-food solar dryer*

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TCSBS 2014

November, 15 - 18, 2014

University of Sidi Bel Abbas, Algeria

<https://sites.google.com/site/huboldtkollegtcbs2014/home>

Program

Program*

* Official language: English

November 15th, 2014

Young Scientist workshop/ training

Participants: 10 PhD students from universities in Algeria

Chairman: Prof. Dr. Hans-Heinrich Limbach (Germany)

Trainers: Prof. Henning Hopf (Germany)

Prof. Dr. Ali Rahmouni (Algeria)

Dr. Derrar Siham (Algeria)

18.00 – 20:00 Registration of the participants to the TCSBS 2014

November 16th:

8:15 Registration of the participants

8:45 Opening session



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- 9:30** **Prof. M. Ellouze (President of the AvH Maghreb association, Sfax, Tunisia):** Presentation of the Alexander von Humboldt-Stiftung
- 9:45** **Dr. Anna Kloska, DAAD lectrice, Oran:** Presentation of the DAAD
- 10:00** **Keynote: Prof. Dr. Michael Springborg (Germany):** response of large systems to static electromagnetic fields
- 10: 45** **Coffee break , Picture of the participants**
- Chairman: Prof. Dr. Hans-Heinrich Limbach (F. Univ.Berlin, Germany)*
- 11:00** **Oral 1: Prof. Dr. Reinhold Fink (Germany):** Quantitative predictions and qualitative insight to exciton mobilities in organic materials by quantum chemical approaches
- 11:30** **Oral 2: Prof. Dr. Yoon Sup Lee (Korea):** Protocols to Calculate Redox Potentials of Transition Metal Complex Ions
- 12:00** **Oral 3: Prof. Dr. Henning Hopf (Germany):** Aromatic Chemistry 150 Years after Kekulé: From the Plane to Three-dimensional Space
- 12:30** **Oral 4: Priv. Doz. Dr. Karin Fink (Germany):** Transition metal compounds in magnetism and catalysis
- 13:00** **Lunch**

Chairman : Prof. Ali Rahmouni (Univ. Saida, Algeria)

- 14:30 Oral 5: Prof. Dr. Belkhiri Lotfi (Algeria):** Relativistic computational study of highly selective N-ligands for Ln(III)/An(III) separation
- 14:50 Oral 6: Prof. Dr. Gérard Vergoten (France):** *A cybernetic approach to molecules, molecular recognition and chemical communication*
- 15:10 Oral 7: Dr. Aurélien Moncomble (France):** Elucidation of metal complex structures by time dependent DFT calculations coupled with electronic spectroscopies
- 15:30 Oral 8: Prof. Dr. Dalila Hammoutène (Algeria):** Computational Molecular Design of Optimal Nonlinear Optical Materials
- 15:50 Coffee break/poster session I**

Chairman: Prof. Dr. Reinhold Fink (Univ. Tuebingen, Germany)

- 16:50 Oral 9: Dr. Sahar Abdalla (Sudan):** Isolated and Deposited Potassium Clusters
- 17:10 Oral 10: Prof. Dr. Marwan Mousa (Jordan):** Microwave Harmonics Generated in Laser-Assisted Scanning Tunneling Microscopy – Their Significance Regarding Terahertz Sources in Laser Assisted Field Emission
- 17:30 Oral 11: Prof. Dr. Aziz Aboulmouhajir (Morocco):** Molecular modeling: petro chemistry and therapeutic chemistry
- 17:50 Oral 12: Prof. Dr. Mourad Lounis (Algeria):** Crash energy dissipation in the head security helmet
- 18:10 Oral 13: Prof. Dr. Mohamed Ellouze (Tunisia):** Critical behavior in manganites in $\text{La}_{0.67}\text{Ba}_{0.22}\text{Sr}_{0.11}\text{Mn}_{1-x}\text{Fe}_x\text{O}_3$ ($0 \leq x \leq 0,2$)

November 17th

Chairman : Prof. Dr. Michael Springborg (Univ. Saarland, Germany)

- 08:30** **Oral 14: Prof. Dr. Hans-Heinrich Limbach (Germany) :** NMR Studies of acid-base interactions: from hydrogen bonded model systems to proteins
- 08:50** **Oral 15: Prof. Dr. Hossein Eslami (Iran) :** Molecular Dynamics Simulation of a Polyamide-Nanotube Nanocomposite
- 09:10** **Oral 16: Prof. Dr. Mohamad El-Khateeb (Jordan):** Organoiron selenocarboxylate Complexes: Synthesis, characterization and Reactivity
- 09:30** **Oral 17: Prof. Dr. Cenk Selcuki (Turkye):** Molecular Modeling of Metal ion interactions with Biochemical Molecules
- 09:50** **Oral 18: Dr. Alberto Del Rio (Italy):** Computational design of bioactive compounds: past, present and future
- 10:10** **Oral 19: Prof. Dr. Abdelkader Souifi (France):**
- 10:40** **Coffee break / Poster Session II**

Chairman : Prof.Dr. Gérard Vergoten (Univ. Lille 1, France)

- 11:40** **Oral 20: Prof. Dr. Ashraf Abadi (Egypt):** Mining ZINC Database to Discover Potential Phosphodiesterase 9 Inhibitors Using Structure-Based Drug Design Approach Industry
- 12:00** **Oral 21: Prof. Dr. Saber Chatti (France):** Synthesis and characterization of polymers from biosourced monomers.



- 12:20** **Oral 22: Prof. Mostefa Belkhatir (Algeria):** Laboratory Study on Static Liquefaction of Overconsolidated Silty Sand Soils: Effect of Sample Preparation
- 12:40** **Oral 23/24/25**
PhD students
- 13:20** *Lunch*

Novembre 18th

Chairman: Prof. Dr. Nasredine Chabane-Sari (Univ. Tlemcen, Algeria)

- 08:30** **Oral 26: Prof. Dr. Sidi Mohammed Mekelleche (Algeria) :** Theoretical study of the mechanism, regio- and stereo-selectivity of cycloaddition reaction
- 08:50** **Oral 27: Dr. Adlane Sayede (France) :** Insight on the ferroelectric properties in (BiFeO₃)₂(SrTiO₃)₄ superlattice: from experiment and ab initio calculations
- 09:10** **Oral 28: Dr. Sami Lakhdar (France):** Phosphido-Boranes: Old Molecules with New Insights
- 09:30** **Oral 29: Prof. Dr. Yasseen Alsoud (Jordan):** Synthesis and Biological Evaluation of Phenyl Substituted 1H-1,2,4-Triazoles as Non-Steroidal Inhibitors
- 09:50** **Oral 30: Prof. Dr. Faouzi Lakrad (Morocco):** Nonlinear vibrations in Atomic Force Microscopy systems



10:10 Oral 31: Dr. Ahmad Telfah (Germany): Online Nuclear Magnetic Resonance (NMR) detection of mass and volume limited living cancer cell and other biological samples

10:30 Coffee break

Chairman: Prof. Dr. Sidi-Mohamed Mekeleche (Univ. Tlemcen, Algeria)

10:50 Oral 32: Prof. Mohamed Hedi Ben Ghazlen (Tunisia): Influences of anisotropy on band gaps of 2D photonic crystal with hexagonal inclusions

11:10 Oral 33: Dr. Samir El Zein (Liban) : Stock markets simulations: from maths to clients

11:30 Oral 34: Prof. Aref Maalej (Tunisia): Performance evaluation of an agrofood solar dryer

11:50 Oral 35: Dr. Ismail Trabelsi (Tunisia): Co-pyrolysis of landfill leachate reverses osmosis concentrate with sewage sludge in a fixed-bed reactor

12:10 Oral 36: Prof. Dr. Latifa Debbi (Algeria): How the study of the fractional Navier-Stokes equation helps in the understanding of the millennium problem

12:30 Oral 37: Dr. Nasser Chellouah (Algeria): Calcined clay in the future cement.

13:00 Lunch

Chairman: Prof. Abdedaim Kadoun (Univ. Sidi Bel Abbès, Algeria), Prof. Dr. Mohamed Ellouze (Univ. Sfax, Tunisia)

14:30 Round table and closing session

Oral presentations



Keynote

The Response of Extended Systems to Static Electromagnetic Fields

Michael Springborg* and Bernard Kirtman**

*Physical and Theoretical Chemistry, University of Saarland, Campus B2.2, 66123 Saarbrücken, Germany

m.springborg@mx.uni-saarland.de

**Department of Chemistry and Biochemistry, University of California, Santa Barbara, California 93106,

USA

kirtman@chem.ucsb.edu

Abstract:

For molecular systems, the quantum-mechanical treatment of their responses to static electromagnetic fields usually employs a scalar-potential treatment of the electric field and a vector-potential treatment of the magnetic field. Although the potential for each field separately is associated with the choice of an (unphysical) origin, the precise choice of the origin for the electrostatic field has little consequences for the results. This is different for the magnetic field where the introduction of so called Gauge-Invariant Atomic Orbitals (GIAOs) poses one approach for removing the origin-dependence of the responses.

For large, extended, regular systems (consisting of a large number of periodically repeated, identical units with deviations from this regularity only at the boundaries) additional problems occur. Thus, for an efficient treatment of such systems, it is practice to treat them as being infinite and periodic. However, the presence of the additional potentials from static electromagnetic fields breaks the translational symmetry. Moreover, these potentials are unbounded.

In the present contribution we shall start with the large, finite, regular system and for this require that a thermodynamic limit exists also when the system is exposed to a static electromagnetic field. This gives information on the properties of the electronic wavefunctions of the system and on its charge distribution. Subsequently, we study the infinite, periodic system with the requirement that the responses of this are identical to those of the large, finite system in its thermodynamic limit. From this requirement, the Hamilton operator for the periodic system is derived. Properties of the resulting single-particle equations are discussed and results of model calculations presented.

Key words: Crystals, Electromagnetic fields, Extended systems, Periodic systems, Responses, Surfaces

OR 01

Applying Computational Chemistry on Material Properties in Organic Electronic Devices

Reinhold F. Fink

Institute of Physical and Theoretical Chemistry, University of Tübingen, Auf der Morgenstelle 18, 72076

Tübingen, Germany

Reinhold.Fink@uni-tuebingen.de

Abstract:

Organic semiconductors play an increasing role as materials in electronic devices such as organic-light-emitting diodes (OLEDs), -solar cells and -field-effect transistors. We present computational chemistry protocols which (i) provide realistic estimates of key parameters of such materials (ii) give atomistic insight into processes limiting material performance and (iii) indicate optimization potentials for this type of devices.

Transport of charge and energy is a key property for organic electronics applications. We present a protocol for transport properties which is based on hopping theory and an efficient solution of the resulting Pauli master equation. Rates for the transfer of electrons, holes or excited states (excitons) between neighbored molecules are evaluated with Marcus theory or with Fermi's golden rule. Quite good performance for exciton and charge transport is demonstrated.

It is well established that inefficient exciton transport is severely limiting the performance of organic solar cells. A comparison of calculated and measured exciton mobilities points to important quenching effects of exciton diffusion. An atomistic picture for exciton trapping was developed on the basis of quantum chemical results. This shows that small motions of neighbored molecules are triggered in excited states of the solid state material leading to deexcitation processes which are supposed to stop further exciton transport. As this quenching mechanism is a strong function of the flexibility and the mutual orientation of the organic molecules within their crystalline or semi-crystalline environment there is a good chance to find materials with better exciton transport properties.

Finally we demonstrate that material layers with deuterium substituted substances may lead to improved performance of organic optoelectronic devices.

Key words: Organic semiconducting materials, solar cells, charge and exciton transport in organic materials.

OR02

Protocols to Calculate Redox Potentials of Transition Metal Complex Ions

Hyungjun Kim and Yoon Sup Lee

Department of Chemistry, KAIST, Daejeon, 305-701, Korea

yslee@kaist.edu

Abstract:

Density functional theory (DFT) calculation has been performed to calculate the redox potential and to predict the correct ground spin state of iron complexes in acetonitrile solvent. Widely used B3LYP functional is applied with the spin state corrected basis sets. The newly developed protocol for the set of 21 iron complexes is to optimize the structure at the level of the B3LYP/6-31G* and to calculate the single point electronic energy with the same functional and the modified basis sets s6-31G* for the iron atom and the 6-31+G* for the other ligand atoms. The solvation energy is considered through the polarized continuum model (PCM) and the cavity creation energy is included for the accurate spin state description. Modifying the cavity size by employing the different scaling factor according to the mean absolute of the natural population analysis charge is introduced. This protocol gives only 1 wrong ground spin state among the 18 iron complexes for which experimental data are known. For the open circuit voltage (OCV) calculation, our protocol performs well yielding the mean absolute error (MAE) of 0.112V for the test set. The close correlation between the calculated and the experimental OCV are obtained. The agreement with experiment is comparable to another method by Galstyan and coworkers utilizing modified functionals and empirical parameters. The present protocol is also applicable to substituted derivatives of the Fe(bpy)₃ complex ions. Other protocols developed for the redox potentials of transition metal ions in aqueous solutions will also be presented.

Key words: OCV of Flow Redox Battery, Redox Potential Calculation, Redox Potential of Metal Complexes, Solvation Energy Calculation.

OR 03

Aromatic Chemistry 150 Years after Kekulé: From the Plane to Three-dimensional Space

Henning Hopf

Technische Universität Braunschweig, Hagenring 30, D-38106 Braunschweig –Germany-

H.Hopf@tu-bs.de

Abstract:

For more than 100 years aromatic chemistry meant the chemistry of planar compounds, i. e. derivatives of benzene, the structure of which Friedrich August Kekulé had established in 1865, following a concept that had appeared to him in a dream.

Today aromatic chemistry is strongly concerned with non-planar, three-dimensional aromatic structures. These may be built of classical planar ring systems or distorted benzene rings. Non-planar aromatics are quickly becoming of importance as ligands in stereoselective synthesis, but also as monomers in polymer chemistry and in material science. The lecture will discuss the most important recent developments in synthesis and application of non-planar aromatic compounds.

Key words:

OR 04

Transition metal compounds in magnetism and catalysis

Karin Fink

Institute of Nanotechnology, Karlsruhe Institute of Technology, Germany

Karin.fink@kit.edu

Abstract:

Transition metal compounds are widely used in technical applications because of their magnetic and catalytic properties. One of the key topics in magnetism is the development of new materials for single molecule magnets (SMMs). On the example of trinuclear transition metal compounds we will show how the magnetic properties can be calculated and analyzed by quantum chemical methods. For this purpose, we perform ab initio calculations on the low energy spectrum of the full electronic Hamiltonian of the trinuclear complexes and determine the interaction of the electronic states with an external magnetic field by finite perturbation theory. With the help of calculations on mononuclear and binuclear model complexes which are constructed by diamagnetic substitution of spin centers the magnetic properties of the polynuclear complexes are traced back to the properties of the individual spin centers (spin multiplicity and zero field splitting) and the interaction of pairs (magnetic exchange coupling J) by effective spin Hamiltonians.

In the field of transition metal catalysis, we investigate asymmetric addition reactions of dialkylzinc to α,β -unsaturated aldehydes catalyzed by [2.2] paracyclophane-based ligands. Quantum chemical calculations were performed to gain insight in the stereo- and regio-selectivities of the reactions. Based on these calculations the differences between cinnamaldehyde and N-formylbenzylimine could be explained. The accuracy of DFT (density functional theory) calculations with different functionals and the influence of dispersion corrections are validated by LPNO-CEPA (local pair natural orbitals coupled electron pair approach) calculations.

Key words: ab initio calculations, transition metal compounds, magnetism, spin orbit, catalysis

OR 05

Relativistic computational study of highly selective *N*-ligands for lanthanides(III)/actinides(III) separation

Lotfi Belkhiri^{*}, Abdellah Zaiter^{*}, Yamina Bouzidi^{*}, Michel Ephritikhine^{**} and Abdou Boucekkine^{***}

^{*}*Unité de Recherche Chimie de l'Environnement et Moléculaire Structurale (URCHEMS), Université de Constantine 1, 25017 Constantine, Algérie*

lotfi.belkhiri@umc.edu.dz ; hizairter@yahoo.fr ; yamina.bouzidi@gmail.com

^{**}*IRAMIS, UMR 3299 CEA/CNRS SIS2M, CEA/Saclay, 91191 Gif-sur-Yvette, France*

michel.ephritikhine@cea.fr

^{***}*Laboratoire Sciences Chimiques de Rennes, UMR-CNRS 6226, Université de Rennes 1, Campus de Beaulieu, 35042 Rennes Cedex, France*

abdou.boucekkine@univ-rennes1.fr

Abstract:

The chemistry of lanthanides (Ln) and actinides (An) species has experienced an extensive growth during the past two decades¹. However, the use of f-elements, e.g. actinides as a nuclear fuel for energy needs, has resulted in an accumulation of contamination issues, including reprocessing and nuclear waste storage.² This originates from the long-lived (>10³ years) radioactive elements such as americium (Am) and curium (Cm) present in spent nuclear fuel. The main remediation issue is the removal of these minor actinides (Am, Cm) by their partitioning from lanthanide elements (fission products) using selective reagents. Among them, polyazines have emerged as highly selective ligands towards actinides over lanthanides ions. Considerable efforts have been thus devoted at both experimental and theoretical levels, to the design, synthesis and developing of these soft *N*-donor ligands in order to carry out the challenging Ln(III)/An(III) separation.³

Theoretical studies are still essential to understand the molecular basis of the observed separation and the different factors, electronic, steric or energetic which can account in favor of the actinide-polyazine selectivity.

In this context, a relativistic computational study using DFT/ZORA approach, was carried out to model Ln(III)/An(III) differentiation, with a special emphasis on the coordination modes of mono- and polyazine complexes, and on the role of f electrons in metal-ligand bonding. Structural,

electronic and energetic analysis, in agreement with experimental finding, reveal that the selectivity of soft *N*-donor ligands to An(III) over Ln(III) may originate from the slightly greater covalent character in An-L bonds with a significant 5f actinide orbitals contribution. DFT/ZORA approach was also found to properly describe the influence of the steric and orbital effects on the selective polyazine complexation on the Ln(III)/An(III) couple.

Keywords: Ln(III)/An(III) differentiation, DFT/ZORA, 5f orbital, covalence, polyazine.

References:

1. (a) Ephritikhine, M., *Dalton Trans.* **2006**, 2501-2516. (b) Edelmann, F.T. *Coord. Chem. Rev.* **2011**, 255, 1834-1920. (c) Fortier, S.; Walensky, J. R.; Wu, G.; Hayton, T. W., *J. Am. Chem. Soc.* **2011**, 133, 6894–97.
2. (a) Dam, H.H. ; Reinhoudt, D.N.; Verboom. W., *Chem. Soc. Rev.*, 2007, 36, 367–377 (b) Lewis, F.W.; Harwood, L.M.; Hudson, M.J.; Drew, M.G.B.; Hubscher-Bruder, V.; Videva, V.; Arnaud-Neu, F.; Stamberg, K.; Vyas, S., *Inorg. Chem.*, **2013**, 52, 4993–5005.
3. (a) A. Zaiter, A. Boudersa, Y. Bouzidi, L. Belkhiri, A. Boucekkine, M. Ephritikhine. *Inorg. Chem* **2014**, *53*, 4687–4697

OR 06

A Cybernetic Approach to Molecules, Molecular Recognition and Chemical Communication

Gérard Vergoten

UGSF, Unité de Glycobiologie Structurale et Fonctionnelle, UMR CNRS 8576

Université Lille 1 Sciences et Technologies - Cité Scientifique - Bâtiment C9 59655 Villeneuve d'Ascq Cedex

– FRANCE-

gerard.vergoten@univ-lille1.fr

Abstract:

Long time Molecular Dynamics simulations based on the home made SPASIBA spectroscopic empirical potential energy function and parameters, partial atomic charges deduced from high level quantum chemical computations and the resolution of the Maxwell equations have been used to propose a novel description of molecules in terms of two characteristics of a communication antenna, i.e. electromagnetic power and directivity. Molecular Recognition and Chemical Communication are interpreted on the basis of the laws of Biocybernetics and the Shannon paradigm in the mathematical theory of communication. Typical molecular systems are pheromones and fragrance molecules which can be easily studied in vacuo. For the molecule-molecule, cell- molecule and cell-cell recognition, some selected amino-acids (arginine, glutamic acid) and glycans (biantennary, triantennary and tetraantennary) are investigated.

Key words: Molecular Dynamics simulations, SPASIBA spectroscopic empirical potential energy, quantum chemical computations Maxwell equations.



OR 07

Elucidation of metal complex structures by TD-DFT calculations coupled with electronic spectroscopies

Aurélien Moncomble and Jean-Paul Cornard

LASIR – Université Lille 1 – Villeneuve d'Ascq, France

aurelien.moncomble@univ-lille1.fr

jean-paul.cornard@univ-lille1.fr

Abstract:

Quercetin is one of the most encountered flavonoid in the vegetation. Owing to its structure that presents three different chelation sites, it can be involved in complexation reactions with many metal cations. Understanding these interactions in solution is important to have insights in their occurrence in the biological medium.

While the interaction between quercetin and several ions have been studied before, a single complex was always identified as the major species.

In this study, we present mainly the quercetin-magnesium(II) system, some results about the quercetin-zinc(II) system will also be evoked. It has been studied by a strong association between electronic spectroscopy measurements (UV-vis absorption, fluorescence) and TD-DFT computations. The comparison between the computed data and the measured ones allowed to show the existence of an equilibrium between two complexes involving two sites of quercetin.

This necessitated the development of a peculiar methodology associating variable-temperature study and a quantitative treatment of the data, deeply rooted in the knowledge acquired by the TD-DFT computations.

Above the fact that it allowed to show the first example of equilibrium between two different complexes on a sole multi-site ligand, the methodology proposed here can be extended to the study of more complex systems involving several species.

Key words: Complexes, Electronic spectroscopies, Quercetin, TD-DFT.



OR 08

Computational Molecular Design of Nonlinear Optical Materials

Dalila Hammoutene

*Laboratoire de Thermodynamique et Modélisation Moléculaire, USTHB BP 32, El Alia 16111 Bab Ezzouar,
Alger, Algeria*
dhammoutene@yahoo.fr

Abstract:

Nonlinear optical (NLO) materials have been the focus of intensive investigations for several decades from both the fundamental and practical points of view for their possible applications in the domain of optoelectronics and photonics. NLO activity can be found in inorganic crystals but also in organic materials. The latter have attracted great interest, owing to their fast and large nonlinearities and to their inherent tailorability, which allows fine-tuning of the NLO properties.

About 20 years ago, the field of NLO was extended to molecular materials featuring organometallic and coordination complexes. Compared to organics, metal-based chromophores offer additional advantages due to their structural, electronic, and optical properties. Greater design flexibility can be achieved by varying the metal, its oxidation state, the ligand environment, and the geometry. In addition, many complexes are known to possess low-lying charge-transfer transitions such as intra-ligand (ILCT), metal-to-ligand (MLCT), and ligand-to-metal (LMCT), which can be associated with large 2nd order nonlinearities β . Metal complexes of nitrogen heterocyclic ligands, represent an important class of NLO chromophores which have received much attention during the last 15 years.

In particular, the molecular quadratic polarizabilities of donor-substituted pyridine and stilbazole metal complexes have been studied by several groups. We have been involved for the past 10 years in the NLO properties of bipyridyl metal complexes. We have previously shown that ligands such as donor-substituted bipyridyl are excellent building blocks for the construction of either dipolar compounds or nondipolar metal complexes of D_3 and D_{2d} symmetry. We have shown that the NLO response is dictated by the intense intra-ligand charge-transfer (ILCT) transition from

the donor group to the acceptor one, and the role of the metal fragment is that of an inductive acceptor. The quadratic NLO properties of octupolar D3 metal complexes of type (II) have also been investigated with other metal ions such as Fe^{II} , Ru^{II} (d^6), Ni^{II} (d^8), and Cu^{II} (d^9). These works have underlined the important role of the metallic core not only as a template but also for its direct participation in the quadratic NLO responses and suggested that other factors such as the geometry of the complexes and the low-energy MLCT transitions may also contribute to the global NLO activity.

Key words: NLO, organics, organometallics, quantum calculations.



OR 09

Isolated and Deposited Potassium Clusters

Sahar Abdalla^{*}, Michael Springborg^{**} and Yi dong^{**}

^{}University of Khartoum, Faculty of Science, Dept. of Chemistry, P.O.Box 321 Khartoum, Sudan*

Sahar.abdalla@uofk.edu

*^{**}Physical and Theoretical Chemistry, University of Saarland, 66123 Saarbrücken, Germany*

m.springborg@mx.uni-saarland.de

y.dong@mx.uni-saarland.de

Abstract:

The energetic and structural properties of isolated potassium clusters as well as such clusters deposited on potassium surface have been investigated. The global total-energy-minima structures of isolated clusters have been determined by using the Density Functional Tight Binding method (DFTB) combined with genetic algorithms. For the isolated clusters in the gas phase, the binding energy, stability function, and structural similarity have been analyzed. Moreover, the overall shape of the clusters and the radial distribution of the atoms have been studied. Subsequently, we have studied the changes in the structural and energetic properties of potassium clusters after they have been deposited softly on (100) and (110) surfaces of a potassium crystal. We have compared the structures of clusters before and after deposition as well as the structures of the clusters on two different surfaces by using the similarity function, and we found that the structures are changed significantly from the gas phase structures. Moreover, the clusters with the same size have different structures on the two surfaces.

Key words: global minima, similarity function, stability function, deposition.

OR 10

Microwave Harmonics Generated in Laser-Assisted Scanning Tunneling Microscopy—Their Significance Regarding Terahertz Sources in Laser Assisted Field Emission

Mark J. Hagmann* and Marwan S. Mousa**

* *NewPath Research L.L.C., Salt Lake City, Utah U.S.A.*

** *Dept. Physics, Mu'tah University, Al-Karak, Jordan*

mhagmann@newpathresearch.com

mmousa@mutah.edu.jo

Abstract:

Recently microwave frequency combs have been generated in the tunneling current of a scanning tunneling microscope (STM) by focusing a mode-locked ultrafast laser on the tunneling junction [1]. These combs are generated by optical rectification to give a waveform that is the envelope of the optical waveform from the laser, with hundreds of measurable harmonics at integer multiples of the pulse repetition frequency of the laser. The harmonics set the present state-of-the-art for narrow linewidth microwave sources. For example, the 200th harmonic, at 14.85 GHz, has a linewidth of less than 1 Hz and a signal-to-noise ratio of 20 dB.

Fourier analysis shows that the periodic sequence of 15 fs pulses in the tunneling current requires that the comb continues to above 30 THz within the tunneling junction. The measured roll-off in the amplitude of successive harmonics has been shown to be caused only by the shunting capacitance of the tunneling junction in the STM—which would be mitigated in laser-assisted field emission. Furthermore, simulations [2] confirmed by recent measurements [3] show that bursts of electrons having a duration of less than 10 fs may be produced by laser-assisted field emission. Thus, the designs we proposed earlier [4] for wide-band tunable terahertz sources are now reconsidered. Our recent developments including robust nanofabricated field emitters operating in air and the use of capacitive ballasting to obtain extremely high-amplitude oscillating field emission currents are included in a second set of designs which we propose for terahertz applications.

Key words: microwave sources, tunable terahertz sources, terahertz applications, ultrafast laser.



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OR 11

Synthesis of Some New Biologically Active Heterocyclic Compounds From Laboratory Available Nitrile Intermediates

Fathy M. Abdelrazek

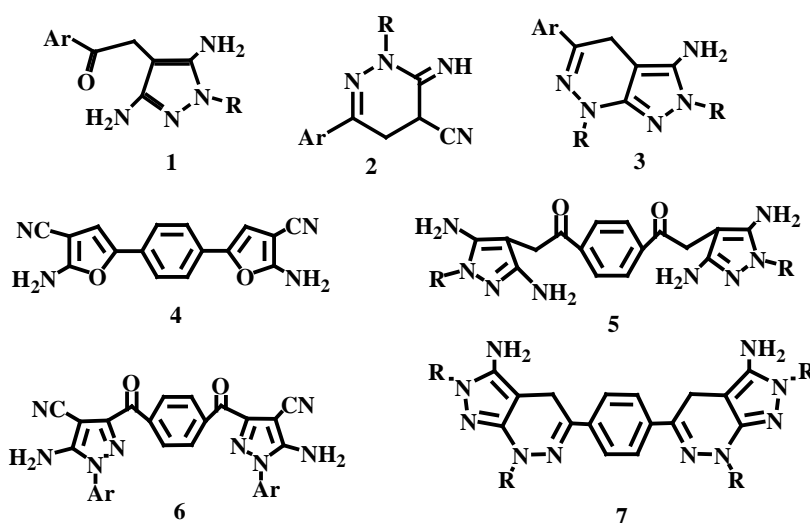
Chemistry Department, Faculty of Science, Cairo University, Giza, Egypt

prof.fmrzek@gmail.com

Abstract:

In continuation of a program aiming to develop new simple routes for the synthesis of heterocyclic compounds of biological interest [1-2] some newly substituted pyrazoles. Pyridazines and their fused derivatives as well as some phenylene 1,4-bis pyrazoles and pyrazolo-pyridazine derivatives were required for biological activity studies. Thus we report in this presentation the synthesis of some novel heterocyclic compounds type 1-8. Some plausible mechanisms will be discussed [3,4].

Key words: Heterocyclic synthesis, Pyridazines, Pyrazolopyrimidines, Bis-heterocycles.



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OR 12

Crash energy dissipation in the head security helmet

Lounis Mourad^{*}, Bessai Naimaa^{*} and Baumgartner Daniel^{**}

^{} Analysis and Application of Radiation Laboratory Department of Physics – Faculty of Sciences – USTOMB
University of Sciences and Technology of Oran BP 1505 El M' Naouer 31000 Algeria*

loumou2000@yahoo.fr

*^{**} Institute of Fluids and Solids Mechanics – University of Strasbourg – France*

Abstract:

The road safety is very important in our social and economic modern life. During an accident, the helmet is the most protective system of the head. The main function of the helmet is to reduce and prevent the human head injuries may occur during a hard impact. It protects the head by absorbing an important part of the crash energy. Principally, in the road security, the energy caused by the high speed arrives at the helmet just before the impact as a kinetic form. When the greater part of energy is absorbed by the deformation and the destruction of the helmet structures, the head will be better protected. We can also consider that the kinetic energy of the different structures of the helmet as another type of energy dissipation witch decrease the head injury. This work proposes an analytic analysis of the mechanical behavior of the different helmet structures with the industrial conditions as the velocity and the mass structures values. Each part of the helmet is represented and assimilated to the association of three elements, a mass, a spring and a dashpot. Each layer is defined by the specific combination of the three elements values.

By evaluating the different kinetic, elastic and viscous energies at each instant after the impact, we can optimize the helmet for a maximum comforts and maximum head security. This energetic evaluation reveals that for more than some values of the velocities the helmet is damage by modifying the structures and limits the helmet validity.

Key words: Crash, Impact, Helmet, Injuries, Tolerance limits.



OR 13

Critical behavior in manganites in $\text{La}_{0.67}\text{Ba}_{0.22}\text{Sr}_{0.11}\text{Mn}_{1-x}\text{Fe}_x\text{O}_3$ ($0 \leq x \leq 0.2$)

M. Ellouze^{*}, S. Mahmood^{**}, F. Ben Jemma^{*}, H. Elkebir^{**} and F. Elhalouani^{***}

^{*}*Université de Sfax, Faculté des Sciences de Sfax, B.P. 1171, Sfax 3000, Tunisie*

^{**}*Université de Jordanie, Amman, Jordanie*

^{***}*Institut Néel, BP 166, F -38042 Grenoble Cedex 9, France*

Mohamed.Ellouze@fss.rnu.tn

El-Kebir.Hlil@neel.cnrs.fr

Résumé

The essential properties of the perovskite $\text{La}_{0.67}\text{Ba}_{0.22}\text{Sr}_{0.11}\text{Mn}_{1-x}\text{Fe}_x\text{O}_3$ ($0 \leq x \leq 0.2$) around the ferromagnetic-paramagnetic transition phase were investigated using modified Arrott and Kouvel Fischer method on the basis of data recorded static magnetic measurements around the Curie temperature (T_C).

Based on the measured critical exponents for the compounds having different values of x ($0.378 \leq \beta \leq 0.411$, $1.247 \leq \gamma \leq 1.393$ et $4.018 \leq \delta \leq 4.73$), we concluded that the transition from paramagnetic-ferromagnetic phase in the compound with $x = 0$ belongs to the three-dimensional Heisenberg universality. However, the substitution of Fe^{3+} to Mn^{3+} the displacement caused in the value of γ to the 3D-model Ising and a slight increase in β . This could be explained by random dilution subnet Mn^{3+} by Fe^{3+} and the removal of the double exchange interaction.

Keywords: perovskite manganite, the critical behavior, isothermal magnetization

OR 14

NMR Studies of acid-base interactions: from hydrogen bonded model systems to proteins

Hans-Heinrich Limbach

Institut für Chemie und Biochemie, Freie Universität Berlin, Takustr. 3, D-14195 Berlin, Germany

limbach@chemie.fu-berlin.de

Abstract:

Using a combination of low-temperature liquid-state and solid-state NMR spectroscopy, combined with recently developed correlations relating hydrogen bond geometries and NMR parameters we have studied functional hydrogen bonds in the active sites of enzymes as well as of suitable model systems. Localization of protons in acid-base hydrogen bonds yields interesting information about the local environment and about the way how an enzyme catalyses biochemical reactions. Examples stem from alanine racemase, aspartate aminotransferase and human carbonic anhydrase II. For further reading see <http://userpage.chemie.fu-berlin.de/~limbach/> (go to "Publications").

I thank my colleagues and coworkers, Shasad Sharif, Monique Chan-Huot, Benjamin Koeppel, Alexandra Dos, Ilya G. Shenderovich, Peter M. Tolstoy, Gleb S. Denisov, Gerd Buntkowsky, Michael Toney, David N. Silverman for their collaboration.

Key words: NMR spectroscopy, Hydrogen bonds, Tautomerism, Enzyme catalysis.

OR 15

Molecular Dynamics Simulation of a Polyamide-Nanotube Nanocomposite

Hossein Eslami

Department of Chemistry, College of Sciences, Persian Gulf University, Boushehr 75168, Iran

`h.eslami@theo.chemie.tu-darmstadt.de`

Abstract:

In this work, oligomeric polyamide-6,6 (PA-6,6) chains, are simulated at the interface of carbon nanotubes (CNTs) of different diameters and the effect of surface curvature and surface area on the structure and dynamics of polymer is studied. Analysis of hydrogen bonding in PA-6,6 at the interface shows that the density of hydrogen bonds (HBs) at close proximity of the CNT surface is less than the corresponding bulk value. This is shown to be due to the energetically favorable orientation of methyleneamide groups of polymer parallel to the CNT surface. However, at distances over which organized layered structures are formed, the number of stronger HBs, compared to the bulk sample, is increased. Very close to the CNT surface the monomers wrap around the tube. The wrapping costs higher energies at the interface of more curved CNT surfaces. The length scale over which the surface effects can perturb the polymer structure depends on the length scale of the structural property of interest. Local structural properties are affected up to a distance of ≈ 2 nm from the surface. However, the CNT surface influences the global chain properties up to distances as long as a few times the radius of gyration of the unperturbed chain.

Due to the formation of extended conformations at the interface, the chain translation at the interface is found to be anisotropic. The magnitude of dynamics deceleration caused by the CNT surface depends on the surface proximity, surface curvature, and the time scale of the unperturbed dynamical property of interest. The dynamics decelerates more in the case of long-time dynamical properties for chains at closer distances to flatter CNT surfaces.

Key words: interphase thickness, nanocomposites, polyamide-6,6, simulation, surfaces and interfaces.

OR 16

Organoiron Selenocarboxylate Complexes: Synthesis, characterization and Reactivity

Mohammad El-khateeb

Chemistry Department, Jordan University of Science and Technology, Irbid 22110 jordan

kateeb@just.edu.jo

Abstract:

Selenocarboxylato complexes of iron containing heterocyclic group of the general formula $\text{CpFe(CO)}_2\text{SeCO-het}$, **1** [het = 2-C₄H₃S (**a**), 2-C₄H₃O (**b**), -CH₂-2-C₄H₃S (**c**)] were made from the reaction of iron selenide, $(\mu\text{-Se})[\text{FeCp(CO)}_2]_2$ and het-COCl. These complexes react with the ligands ER₃ (E = P, R = Ph, OC₂H₅; E = As, Sb, R = Ph)] under photolytic conditions to give the monosubstituted complexes $\text{CpFe(CO)(ER}_3\text{)SCO-het}$ **2-5** in good yields. The new complexes have been characterized by elemental analysis, IR and ¹H NMR spectroscopy. The solid state structure of $\text{CpFe(CO)}_2\text{SeCO-2-C}_4\text{H}_3\text{S}$, has been determined by X-ray crystal structure analysis.

Key words: Complexes, Iron, Selenocarboxylates, Structures, Substitution.

OR 17

Molecular Modeling of Metal Ion Interactions with Biochemical Molecules

Cenk Selçuki

Ege University, Faculty of Science, Biochemistry Department 35100 Bornova/Izmir/Turkey

cenk.selcuki@ege.edu.tr

Abstract:

Some metal ions are essential for living cells. They mainly act as co-factors for metalloproteins; but, they are also potentially toxic when their concentrations exceed tolerated limits. Recent studies indicate that some metal ions also play important role in metabolic process regulations. This work will summarize some of the model systems investigated in our group in order to understand the mechanism(s) of metal ion-biomolecule interactions by using computational tools, mainly quantum chemical techniques based on Density Functional Theory (DFT). A better understanding of the interaction mechanisms not only will enable us to minimize the effects of metal toxicity but also will help us to improve new hybrid systems that can be used in many different fields from health to bionanotechnology. Our preliminary results indicate that metal ions mostly bind to specific sites with a high selectivity in the studied model systems.

Key words: Molecular Modeling, Metal Ion, Peptide, Amino acid, Density Functional Theory

OR 18

Computational design of epigenetic drugs: past, present and future

Alberto Del Rio^{*,**}

** Institute of Organic Synthesis and Photoreactivity (ISOF), National Research Council (CNR)*

Via P. Gobetti 101, 40129 Bologna, Italy

*** Department of Experimental, Diagnostic and Specialty Medicine (DIMES), Alma Mater Studiorum,*

University of Bologna, Via S. Giacomo 14, 40126 Bologna, Italy

alberto.delrio@isof.cnr.it

alberto.delrio@gmail.com

Abstract:

The study of epigenetic mechanisms, including DNA methylation, different forms of histone post-translational modifications (PTMs) and gene expression by non-coding RNAs, marked an extraordinary progression in the last years and many of them have been identified and associated to different fundamental biological processes and pathological conditions. Consistently, several drug discovery programs aimed to devise small-molecules able to pharmacologically modulate epigenetic targets have been initiated.

Computer-aided molecular design techniques still constitute an effective set of tools to guide the selection of new compounds with predefined biological activity. These techniques include a variety of chemoinformatic and computational chemistry tools. In particular, virtual screening procedures are well established for the rapid and cost-effective evaluation of large chemical libraries of compounds. The growing availability of three-dimensional structures of epigenetic targets raised the possibility to deploy structure-based drug design techniques, like docking or pharmacophore screenings, in search of novel compounds able to modulate these targets.

Herein we provide a past, present and future overview of molecular design approaches to target epigenetic proteins, with a particular focus on those that emerged as important targets for cancer therapy. We will present two typical computer-aided approaches that have been used to identify novel inhibitors of SIRT6, a member of the NAD⁺-dependent histone deacetylases, and SMYD3, a member of the histone lysine methyltransferases.

Key words: Cancer therapy, Computer-aided molecular design, Drug design, Epigenetics.



OR 20

Mining ZINC Database to Discover Potential Phosphodiesterase 9 Inhibitors Using Structure-Based Drug Design Approach

Ashraf H. Abadi*, Engi A. Hassan* and Gary A. Piazza**

*Department of Pharmaceutical Chemistry, Faculty of Pharmacy and Biotechnology, German University in Cairo, Cairo 11835, Egypt

**USA Mitchell Cancer Institute 1660 Springhill Avenue, Alabama 36604, United States
ashraf.abadi@guc.edu.eg

Abstract:

A structure-based drug discovery approach was undertaken to mine the ZINC database for virtual screening to identify novel PDE9 inhibitors. The database was screened against the ligand binding pocket of the PDE9 complex (PDB:4GH6) using molecular docking programs, MOE and AutoDock Vina in PyRx. This led to the discovery of three novel scaffolds that potently and selectively inhibit PDE9. Consistent with a role of PDE9 in cancer cell growth, the compounds inhibited also the growth of breast tumor cells at concentrations that inhibit PDE9. A pharmacophore model is proposed for chemical optimization.

Key words: Drug design, PDE9, Phosphodiesterase inhibitor, ZINC database.



OR 22

Laboratory Study on Static Liquefaction of Overconsolidated Silty Sand Soils: Effect of Sample Preparation

Youcef Mahmoudi^{*}, Abdellah Cherif Taiba^{*}, Mostefa Belkhatir^{*,**} and Tom Schanz^{**}

^{*}Laboratory of Material Sciences & Environment, University of Chlef (Algeria)

^{**}Laboratory of Foundation Engineering, Soil and Rock Mechanics, Bochum Ruhr University (Germany)

abelkhatir@yahoo.com

Abstract:

The study of the post-liquefaction stability of earth structures using the undrained shear strength characteristics of silty sand soils that are prone to liquefaction is becoming a major challenge in Geotechnical Earthquake Engineering. The objective of this laboratory investigation is to study the effect of the sample preparation on the undrained shear strength (liquefaction resistance) of medium dense ($D_r = 52\%$) overconsolidated sand-silt mixtures under monotonic loading conditions. For this purpose, a series of undrained monotonic triaxial tests were carried out on reconstituted saturated silty sand samples with fines content ranging from 0 to 40%. The confining pressure was kept constant to 100 kPa in all tests. The samples were prepared using two depositional methods named: dry funnel pluviation and wet deposition for different overconsolidation ratios ($OCR=1, 2, 4$ and 8). The obtained data show that the samples reconstituted with dry pluviation are more resistant than those reconstituted with wet deposition method and that complete static liquefaction of samples reconstituted with wet deposition method was observed in the case of lower overconsolidation ratios. The test results indicate also that for the two depositional methods, the liquefaction resistance increases with the increase of the overconsolidation ratio (OCR) expressed by dilative response tendency increase. The liquefaction resistance decreases with the increase of fines content for dry funnel pluviation and the inverse tendency was observed in the case of wet deposition for the range of the overconsolidation ratio under consideration.

Key words: Overconsolidation ratio, Silty sand, fines content, liquefaction, Dry funnel pluviation, Wet deposition.

OR 26

Theoretical study of the mechanism, regio- and stereoselectivity of cycloaddition reactions

Sidi Mohamed Mekelleche

Laboratory of Applied Thermodynamics and Molecular Modelling, Department of Chemistry, Faculty of Science, University of Tlemcen, PB 119, Tlemcen, 13000, Algeria

sidi_mekelleche@yahoo.fr & sm_mekelleche@mail.univ-tlemcen.dz

Abstract:

In this contribution, we present recent theoretical approaches used for the study and analysis of the mechanism, regio- and stereoselectivity of some cycloaddition reactions, namely,

- i) the intermolecular Diels-Alder reaction of isoprene with acrylic acid in the presence of the 1-ethyl-pyridinium trifluoroacetate ionic liquid.
- ii) the intramolecular Diels-Alder reaction yielding to the formation of the 5aH-chromeno[2,3-c]acridine in the presence of BF₃ lewis acid catalyst and acetonitrile solvent.
- iii) the 1,3- dipolar cycloaddition of α -aryl nitrene with methacrolein in dichloromethane solvent.

Key words: Cycloaddition reactions, Diels-Alder reaction, Molecular mechanism, Regioselectivity; Stereoselectivity, Solvent effects, Quantum chemistry calculations.



OR 27

Insight on the ferroelectric properties in (BiFeO₃)₂(SrTiO₃)₄ superlattice: from experiment and ab initio calculations

A. Sayede, E. Bruyer and R. Desfeux

Univ Lille Nord de France, F-59000 Lille, France

UArtois, UCCS, F-62300 Lens, France

CNRS, UMR 8181, F-59650 Villeneuve d'Ascq, France

Adlane.sayede@univ-artois.fr

Abstract:

Ferroelectric domains properties of (BiFeO₃)₂(SrTiO₃)₄ superlattice were studied by means of piezoresponse force microscopy and density functional theory calculations. A combination of out-of-plane and in-plane piezoresponse force imaging confirms the ferroelectric domains are oriented along the out-of-plane [001] direction of the film. Density functional theory calculations evidence that this orientation is due to the tetragonal-like structure adopted by the BFO units inside the superlattice in response to the interfacial strains. On the other hand, the much lower coercive voltage measured on superlattice compared to BiFeO₃ single layer suggests a more reliable switching capability. The results will bring an insight in the understanding of functional oxide superlattices.

Key words: DFT, ferroelectric properties, multiferroic, PFM.



OR 28

Phosphines–boranes : Old Molecules with New Insights

Roman Gritcenko^{*}, Jacques Lalevée^{**}, Annie–Claude Gaumont^{*} and Sami Lakhdar^{*}

^{*} *Laboratoire de Chimie Moléculaire et Thio-organique, UMR CNRS 6507, 6, boulevard du Maréchal Juin,
14050 CAEN*

^{**} *Université de Haute-Alsace, 2, rue des Frères Lumière, F-68093, Mulhouse*

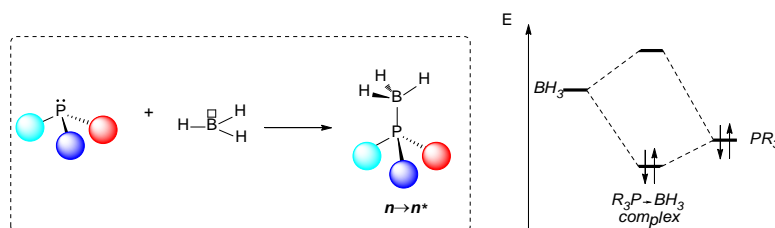
Annie-claude.gaumont@ensicaen.fr

Sami.lakhdar@ensicaen.fr

Abstract:

Lewis acid-Lewis base association has become one of the most important modes of activation in modern organic chemistry.^[1] Based on this concept, various reagents have been developed and found wide application in synthesis.^[2] For instance, carbene-boranes have recently been shown to exhibit excellent reactivity in ionic, radical, organometallic and photopolymerization.^[4] In contrast, phosphine-boranes are known to be reactive in radical reactions,^[3] but not effective enough in ionic reactions.

As part of our efforts to develop a new generation of reactive phosphine-boranes, we present in this communication a new class of molecules exhibiting extraordinary hydrides reactivity in both radical and ionic reactions. Quantification of the hydricity of these molecules as well as elucidation of their molecular structures in solution and in solid state will be discussed.



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OR 29

Synthesis and Biological Evaluation of Phenyl Substituted 1H-1, 2, 4-Triazoles as Non-Steroidal Inhibitors

Yaseen A. Al-Soud* and Rolf W. Hartmann**

* *Department of Chemistry, College of Science, University of Al al-Bayt, Al-Mafraq, Jordan*

** *Helmholtz Institute for Pharmaceutical Science Saarland, Saarland University, Saarbrücken, Germany*

alsoud@aabu.edu.jo

rwh@mx.uni-saarland.de

Abstract:

A series of disubstituted-1H-1,2,4-triazole derivatives were synthesized with the aim of developing new non-steroidal inhibitors of 17 β -hydroxysteroid dehydrogenase type 2 (17 β -HSD2), which might be a novel and attractive target for the treatment of osteoporosis. 17 β -HSD2 catalyses the oxydation of the highly active estrogen 17 β -estradiol (E2) and androgen testosterone (T) into the weak estrone and androstenedione, respectively. Inhibition of this enzyme will lead to a bone local increase in E2 and T levels, two key players in the maintenance of the balance between bone formation and bone formation. In this study, a new class of 17 β -HSD2 inhibitors with a 1H-1,2,4-triazole scaffold has been identified, the best compounds showed moderate 17 β -HSD2 inhibitory activity and a good selectivity toward 17 β -HSD1. They could be a useful tool to map the unexplored enzyme active site.

Key words: 17 β -HSD2/ non-steroidal inhibitor/ osteoporosis/ disubstituted 1H-1, 2, 4-triazoles.

OR 30

Nonlinear Vibrations in Atomic Force Microscopy Systems

Faouzi Lakrad and Mourad Khadraoui

University Hassan II Casablanca, Faculty of sciences Aïn Chock, BP 5366 Maarif, Casablanca, Morocco

lakrad@hotmail.com

morad.khad@gmail.com

Abstract:

We study nonlinear dynamics of a lumped model of an AFM system under the Lennard-Jones forces and a very low frequency base displacement. It is shown that the invariant slow manifolds govern the AFM-modes (contact, noncontact and tapping modes) and the contact duration. The tapping modes are shown to be triggered through two dynamic saddle-node bifurcations.

Key words: Atomic force microscopy, tapping mode, slow manifolds, low frequency, Lennard-Jones forces.



OR 31

Online Nuclear Magnetic Resonance (NMR) detection of mass and volume limited living cancer cell and other biological samples

Ahmad Telfah, Ayten Kalfe, Jörg Lambert and Roland Hergenröder

ISAS - Institute for Analytical Sciences, Bunsen-Kirchhoff-Str. 11, 44139 Dortmund, Germany

telfah.ahmad@isas.de
roland.hergenroeder@isas.de
lambert@isas.de, ayten.kalfe@isas.de

Abstract:

Nuclear Magnetic Resonance (NMR) spectroscopy is a powerful analytical technique with a wide range of applications, and it is a very information-rich and reliable analytical method which gives comprehensive chemical information about the composition of unknown materials. Typical NMR analyses are carried out in 5 and 3 mm sample tubes with approximately 700 – 200 μ L of sample. Measuring small and ultra-small sample volumes is not possible due to the limit of detection (LOD).

A Microstrip NMR detector was designed to enable the investigation of volume-limited samples in the low nanoliter range. Therefore, NMR spectra of sample quantities in the 100 pmol range can be obtained with this microprobe in a few seconds. Moreover, the planar geometry of the detector is suitable for the size and geometry requirements of such a different kind of microfluidic cellular sample holder.

Since NMR is a non-destructive technique with high speciation performance, it is one of the major technologies for metabolic profiling, and it allows in vivo measurements of biological cells.

In our ongoing research, we focus on the metabolic analysis of living human cancer cells; the data obtained on the concentrations and the production \ degradation rates of the metabolites give direct evidence of the present status of the cell, which assists us in the understanding of biochemical pathways. A cellular microfluidic NMR sample holder was designed with a temperature and proper gas atmosphere controlled environment, in order to maintain the viability of the biological cells at near physiological conditions for long-term in vitro studies.

As a near future investigation, living cancer cell samples will be treated with metal-based anti-cancer drugs (e.g. platinum-based drugs). Metabolomics response analysis combined with (^1H , ^{195}Pt) NMR studies (signals and correlation times) will be employed to understand the molecular mechanism of anticancer drug action and to find out the transport mechanism through the cellular membrane. The pseudo-first-order rate constant for the reaction of anti-cancer drugs with water will be defined by a quantitative calculation of the organic and inorganic platinum NMR signal of the treated cells. This rate constant is a very important parameter for monitoring the efficiency, aging and degradation of metal-based anti-cancer drugs.

OR 32

INFLUENCES OF ANISOTROPY ON BAND GAPS OF 2D PHONONIC CRYSTAL WITH HEXAGONAL INCLUSIONS

M.H. Ben Ghazlen, FSS BP 1171 CP 3000 Sfax (Tunisie)

mohhghozlen@gmail.com

We study the band gaps related to a two-dimensional phononic crystal composed with anisotropic cylindrical fillers incorporated in an isotropic matrix. The plane wave expansion method (PWE) is used to reduce the band structure problem to an Eigen value problem. This approach can be generalized to different types of symmetry, and allows the introduction of new physical properties such as piezoelectricity. The square lattice periodic structure is examined. For an hexagonal material implantation in phononic crystal, the band gap depends not only on periodic array but also on the angle between the high symmetry axis and that of the periodic structure. Altering the angle, by rotation of the cylinder, pass bands and forbidden bands of the phononic crystal are changed. For the numerical illustration, one composite of interest has been considered. The localization and width of band gaps are estimated for different implantation factor and for different rotation angle.

The research progress in the area of physical properties of ZnO nanostructures, including mechanical, piezoelectric, electrical, optical, magnetic and chemical leads us to consider phononic materials with ZnO as implantation. We deal with various structures where elastic rods cylinders (ZnO) are embedded periodically in a background material (Epoxy), forming a square lattice. Due to the periodic character of phononic crystals, only the wave vectors k belonging to the first Brillouin zone, are considered for the computation of their band- structures. Thus the Eigen-modes obtained from the motion equation, are either xy modes or z modes, which are completely decoupled since the symmetry is comparatively high.

OR 33

Stock markets simulations: from maths to clients

Samir EL Zein

Sultan Tower, 9th floor, Haddadine street, Abou Samra, Tripoli, Lebanon

samir.el.zein1978@gmail.com

sez@dailyStockSelect.com

Abstract:

Stock markets modeling is a theme attracting more and more theorists around the world for many reasons not the least of which is the daily availability of empirical data (stock prices) as well as the possibility of high rewards (income wise). Daily Stock Select (.com) website was introduced last year in Tunisia as part of the Humboldt college meeting, it was still an ambition and feasible idea. Now the website is up and running for the last 7 Months attracting thousands of users around the world. It offers daily forecasts of the USA markets recommending what stocks to buy expecting their price to raise in the coming week or two. Mathematical research on the random stock prices data include among others Fourier transforms, Hierarchical clustering, Statistical distributions and Linear regression analysis, where every new strategy must be directly tested on the real market before being presented to the web subscribers. Our latest research findings and experience in selling directly to traders will be presented.

Key words: Modeling , Randomness, Statistics, Stock markets simulations.



OR 34

Performance evaluation of an agro-food solar dryer

H. Bentaher, A. Elloumi, H. Chouikhi, R. Kamel, M. Ben Hamouda, N. BENALI A.
Maalej

Labo LASEM, ENIS, University of Sfax, Tunisia

aref.maalej@yahoo.fr

Abstract:

Agricultural products are subject to spoil if not conserved. One of the main problems in the MENA rural region is food conservation due to electricity scarcity. Farmers mainly use drying as a solution to preserve several agro-food products such as tomatoes, chillies, medicinal plants...

However, they mainly used the direct exposition of these products to the sun and that may cause their quality degradation due to dust, UV, etc.

The goal of the European Project ESSORENTPREPRISE is the promotion of agro-food micro-enterprises by the integration of miniaturized machines. In its framework, a solar dryer was designed and constructed. Using a PVT panel, a gain of more than 25°C in temperature was recorded in comparison with the ambient. A dehumidifier, based on a silica gel desiccant bed, was integrated to ameliorate the performances of the drying process. The forced convection of air was studied in several rooms of the dryer by the measurement of the air speed in different points. The obtained results are used to optimize the function of different modes of the dryer as well as to dimension new dryers.

Key words: Solar dryer, PVT, Agro-food, Dehumidifier.



OR 35

Co-pyrolysis of landfill leachate reverses osmosis concentrate with sewage sludge in a fixed-bed reactor

A. Ben Hassen-Trabelsi^{*}, S. Naoui^{*}, E. Ben Amor^{*}, A. Cherbib^{*} and I. Trabelsi^{**}

^{*} *Research and Technology Centre of Energy, Technopôle Borj-Cédria, B.P N°95 2050 - Hammam Lif - Tunisie*

^{**} *Research and Technology Centre of Water, Technopôle Borj-Cédria, B.P N°95 2050 - Hammam Lif - Tunisie*

aida.benhassen@crtten.rnrt.tn

Ismail.trabelsi@certe.rnrt.tn

Abstract:

In Tunisia, the reverse osmosis technique is the most common practice for landfill leachate treatment. The leachate treatment plant generates 30% of the feed as concentrate with high concentration of salts and contaminants. Thus, there is an urgent need for solving the reverses osmosis concentrate problem. The co-pyrolysis of landfill leachate reverses osmosis concentrate (ROC) with sewage sludge (SS) has been investigated in a laboratory scale fixed-bed reactor and the main products (liquid bio-oil, solid bio-char and synthesis gas or syngas) were obtained. In the initial phase, several mixtures of ROC and SS were prepared in order to obtain a slurry mixture with high organic charge and low water content, suitable for thermal treatment. The optimal mixture was pyrolyzed under nitrogen, at different temperatures (450°C, 500°C and 550°C) and at different heating rates (10°C min⁻¹, 15°C min⁻¹ and 20°C min⁻¹). These experiments indicate that the maximum liquid yield (31%) was obtained at the temperature of 550°C and the heating rate of 10°C min⁻¹. The characterization of the pyrolysis products (bio-oil, bio-char and syngas) obtained from co-pyrolysis of the ROC with SS, indicate that they can be used as renewable source energy or as a potential source for synthesis fuels and chemical feedstock. It can be concluded that the pyrolysis as an innovative process could be an alternative for solving the ROC problem.

Key words: landfill leachates, reverses osmosis concentrate, sewage sludge, pyrolysis, bio-oil, bio-char.

OR 36

How the study of the fractional Navier-Stokes equation helps in the understanding of the millennium problem

Latifa Debbi

Department of Mathematics, Faculty of Sciences, University of Boumerdes, Avenue of the Independence, 35000, Boumerdes, Algeria.

Latifa.debbi@gmail.com

This work is supported by Alexander von Humboldt Foundation.

Abstract:

This talk is a reading of the results obtained by the speaker in the work supported by Alexander von Humboldt and entitled: “Well-posedness of the multidimensional fractional stochastic Navier-Stokes equations on the torus and on bounded domains.”

Key words: Fractional Navier-Stokes equation, Navier-Stokes millennium problem, subcritical, critical, supercritical, dissipative and hyperdissipative regimes, Serrin's condition, Beale-Kato-Majda condition.

OR 37

Calcined clay in the futur cement

Nasser Chellouah

nasser_chelouah@yahoo.fr

Abstract:

Currently economical and environmental advantages of cement clinker replacement by other supplementary cementitious materials are well known. For example calcined clays, such as metakaolin, have drawn special attention during recent years. Another option is the development and marketing of completely new cements or cementitious binders and it is well known that these admixtures added to mortars and concretes improve mechanical strength as well as durability. The purpose of this study is to evaluate the behavior of physical-mechanical properties in mortars, by employing calcinated and grinded clays as replacement material, by different percentage of ordinary Portland cement.

Keywords:

Poster presentations



PO 01

Study of the Interaction β -Secretase-Flavonoids by The Molecular Modeling Methods: The Future Treatment of Alzheimer Disease

I.Abdelli, S. Sari and S. Ghalem

University Abou-Bakr Belkaid -Faculty of Science- Department of Chemistry- Laboratory of Natural Substances and Bioactive (LASNABIO)-Tlemcen-Algeria

i_abdelli@yahoo.fr

sari_souad@yahoo.fr

s_ghalem2002@yahoo.fr

Abstract:

β -Amyloid ($A\beta$) peptide has been known to play a crucial role in the development of Alzheimer's disease (AD) because $A\beta$ peptides can form insoluble plaques resulting in severe memory loss and neuronal cell death. $A\beta$ peptides are derived from a sequential proteolytic cleavage of amyloid precursor protein (APP) by β - and γ -secretase. The late limiting step in this process is cleavage of membrane-bound APP by β -secretase to form soluble APP ($sAPP\beta$) and 12 kDa peptide, C99. One way to retard or prevent Alzheimer disease may be to block these secretases, thus preventing proliferation of plaques. For these reasons, the inhibition of β -secretase has become important drug target. With the goal of obtaining the inhibitors of β -secretase, our work consists to study theoretically the interaction β -secretase- flavonoids using the DFT method and molecular docking.

Keywords: β -secretase, flavonoids structure, DFT method, molecular docking.

PO 02

Structures and Properties of Indigo N-Glycosides

K.Adjir and M. Sekkal-Rahal

L2MSM, Faculté des Sciences, Université Djillali Liabes de Sidi Bel Abbès,

B.P. 89, 22000 Sidi Bel Abbès (Algeria).

khadijsaida@yahoo.fr

majsekkal@msn.com

Abstract:

The first deprotected indigo N-glycosides (blue sugars) represent promising anticancer agents, they have been prepared by reaction of dehydroindigo with in situ generated rhamnosyl, glucosyl and mannosyl iodide. The products show a significant anti-proliferative activity against various human cancer cell lines.

In this present work we investigated the grafting of a group of molecules containing two rhamnose's conformations carbohydrates on the indigo molecule. The formation of the compound and its properties as ¹H NMR chemical shifts, vibrational wavenumbers and energies of the optimized structures have been evaluated by quantum chemical calculations using density functional theory (DFT), B3LYP functional and cc-PVDZ as basis set. NBO analysis has been carried out to investigate the stabilization energy of various intra and intermolecular interactions in molecular system. The local reactivity descriptors such as Fukui functions (f^+ , f^-) were performed to determine the reactive sites within the molecule. The study shows that the indigo is very stable due to the large π conjugation inside the molecule along 10 carbon atoms. The electrophilic charge transfer (ECT) confirms the electrophilic behavior of carbohydrate and nucleophilic behavior of indigo. The calculated ¹H NMR chemical shifts are in good agreement with the observed chemical shifts experimentally. The grafting of carbohydrates has effect on indigo's intramolecular distances and this effect depends on the conformation of the carbohydrates, intermolecular distances and the number and type of hydrogen bonds formed between the two molecules. In the gas phase, NBO analysis confirms the presence of inter and intramolecular hydrogen bonds. The intramolecular interactions can be established and can significantly influence overall molecular structures and energetics.

Key words: Anti-proliferative agents, DFT Method, NBO analysis, Indigo N-glycosides.

PO 03

DFT Study of Nucleic Acid Base Pairs Complexes

N.E.-Y. Amraoui and D. Hammoutène

*Laboratory of Thermodynamic and Molecular Modelization, Chemistry Faculty, USTHB, BP32 El Alia,
16111 Bab Ezzouar, Algiers, Algeria.*

amraoui.nour@yahoo.com

dhammoutene@yahoo.fr

Abstract:

Nucleic acids DNA and RNA are polyelectrolyte biological systems having a large number of negative charges on phosphate groups, that's why metal ions and their complexes interact with them. These complexes act as anti-inflammatory and anti-tumor drugs. These interactions of DNA with several natural products, synthetic drugs and drug candidates are known to be metal-mediated. Drug–DNA interactions can be classified into two major categories, intercalation and groove binding.

In this study, we follow a theoretical approach using dispersion-corrected Density Functional methods to evaluate a variety of artificial nucleobases as candidates interacting with some metal ions. We focus on adenine and thymine base pair with $M = \text{Cu(II)}, \text{Co(II)}, \text{Ru(I)}, \text{Ni(I)}$. All calculations are performed using (**ADF 09**) program. Metal-mediated base pairs are studied as drug candidates, their geometry optimizations are performed at **ZORA/TZ2P/BLYP-D** level. The molecular geometries and different energies as total energies, coordination energies, Pauli interactions, orbitalar interactions and electrostatic energies are determined.

Key words: DFT, DNA, DNA-drug interaction, RNA.

PO 04

Ni/SiC-6H Schottky diode for a very sensitive air-pollution detection

Macho Anani*, Mohammed Azzedine** and Mohammed el Hadi Louhibi*,
Zouaoui Chama*, Sara Lebid*, Youcef Amar* and Christian Mathieu***

*Djillali Liabes University. BP 89. 22000. Sidi Bel Abbès. Algeria.

anani66@yahoo.fr

louhibi-meh@yahoo.fr

chama.zouaoui@hotmail.fr

sara0884@yahoo.fr

y_amardz@yahoo.fr

**AbdelHamid Ibn Badis University. 27000. Mostaganem.

azzed@yahoo.fr

***Faculté des Sciences Jean Perrin. Université d'Artois. 62300 Lens. France.

christian.mathieu@univ-artois.fr

Abstract:

Semiconductor junctions have the very interesting property of seeing their impedances be modified in contact with certain gases. This sensitive property is due to the fact that the junction is literally polarized by the gas particles.

Incorporating them into a Wheatstone bridge and calibrating them correctly, such structures would work like gas detectors dedicated to measure precisely the amount and especially the nature or the gas in question.

Also, the Schottky diode has the particularity of being relatively simple in design but also to have the shortest time response compared to other types of junction.

Furthermore, the nature of silicon carbide, this very strong and temperature resistant semiconductor makes it an excellent component for work in particularly hostile and harsh environments.

Keywords: Ni/SiC-6H Schottky diode, Sensor, Air-pollution, modeling



PO 05

Theoretical Study of the Structure and ^1H and ^{13}C NMR Spectrums of Glutaconaldehyde Stereoisomers

T. Ardjani* and S. M. Mekelleche**

*Laboratory of Applied Thermodynamics and Molecular Modeling, Department of Chemistry, Faculty of Science, University A. Belkaid of Tlemcen, PB 119, Tlemcen, 13000, ALGERIA

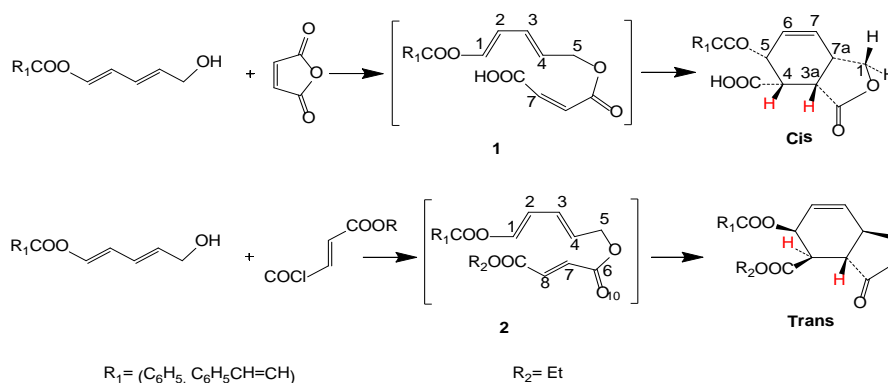
takiainan@yahoo.fr

**Preparing School in Sciences and Techniques of Tlemcen, BP 165 RP Bel Horizon, 13000, Tlemcen, Algeria

sidi_mekelleche@yahoo.fr

Abstract:

Experimentally, it has been found that the intramolecular [4+2] cycloaddition of the glutaconaldehyde derivative substituted by a COOH carboxylic acid group leads to the formation of cis cycloadduct; whereas the substitution by an ester group COOR leads to the trans configuration (Scheme 1).



Scheme 1

In the present contribution, we present a theoretical study of the structure and spectroscopic (^1H and ^{13}C nuclear magnetic resonance chemical shifts and coupling constants) properties of the cis and trans stereoisomers. The calculations were performed at the B3LYP level of theory using the 6-31G(d) and 6-31G(d,p) basis sets and the solvent effects are taken into account using IEFPCM solvation model. The obtained results are in good agreement with experimental findings.

Key words: Glutaconaldehyde, Nuclear magnetic resonance, Chemical shifts, Coupling constants, DFT calculations.

PO 06

Calculation of cross sections by an optical potential method in ESEM: Monatomic gases case

F. Azza *, O.Mansour* and A.Kadoun *

**Faculté des Sciences, Laboratoire L2MSM, Université Djillali Liabes de Sidi Bel Abbès,
B.P.89, Sidi Bel Abbès, 22000, ALGERIA*

Faiza.azza@ymail.com

momaro2002@yahoo.fr

akadoun@yahoo.com

Abstract:

Optimizing imaging conditions in the Environmental scanning electron microscopy (ESEM), needs a detailed knowledge of the microscopic distribution of the interactions, and then the electron density distribution in the skirt, as this might have a decisive effect on the probe profile and hence on the contrast and resolution of the apparatus. Monte Carlo simulations are particularly suitable for this task. However, the development of these simulations requires accurate interaction cross-sections for all the electronic processes and especially the elastic scattering. In this work, an optical potential is used to calculate electron-gas scattering cross sections in the low and intermediate energy range for two monatomic gases, argon and helium. Comparisons are made with experimental and theoretical cross sections used in the literature.

Key words: ESEM, gaseous environment, Optical Potential, Scattering cross section.

PO 07

Structural, electronic and optical properties of BaX (X=S and Te) alloys

K. Babesse*, B. Bahloul**, A. Dekhira*** and D. Hammoutene*

**Laboratory of Thermodynamics and molecular modeling, USTHB, 16000 Algiers*

babessek@yahoo.com

***Material Physics Laboratory, Faculty of Physical Sciences, USTHB, 16000 Algiers, Algeria*

cyber.brahim@yahoo.fr

****Laboratory of Theoretical, Computational Chemistry and Photonics, USTHB, 16000 Algiers*

Abstract:

Structural, electronic and optical properties of BaX (X=S and Te) alloys were calculated using the density functional theory. A pseudopotential plane-wave method as implemented in the ABINIT code. In particular, the lattice constant, energy band gaps, refractive index and dielectric constants are calculated and compared with available experimental and other theoretical values. The dielectric constant and refractive index was studied using different models.

Key words: Ab initio calculations, Electronic properties, Optical constants

PO 08

Ab initio calculations of structural, electronic and thermodynamic properties of BaSrTe alloys

B. Bahloul*, K. Babesse**, A. Dkhira**, Y. Bahloul*** and L. Amirouche*

*: *Material Physics Laboratory, Faculty of Physical Sciences, USTHB, 16000 Algiers, Algeria*

cyber.brahim@yahoo.fr

** : *Laboratory of Theoretical, Computational Chemistry and Photonics, USTHB, 16000 Algiers*

*** : *Department of Materials Science, University of Bordj Bou-Arredj, Bordj Bou-Arredj, Algeria*

Bahloul_1985@yahoo.fr

Abstract:

Structural, electronic and optical properties of BaSrTe alloys were calculated using the density functional theory. A pseudopotential plane-wave method as implemented in the ABINIT code. In particular, the lattice constant, bulk modulus and energy band gaps are calculated and compared with available experimental and other theoretical values. In addition, we have predicted the heat capacities (C_v), the entropy (S), the internal energy (U) and the Helmholtz free energy (F).

Key words: Ab initio calculations, Semiconductors, Electronic properties, Thermodynamic properties.

PO 09

Structural and spectroscopic properties of a complex of vitamin E with vanadyl (II): Insight from ONIOM study

Bakhouché Kahina* and Hammoutène Dalila*

**Laboratoire de Thermodynamique et Modélisation Moléculaire, USTHB BP 32, El Alia 16111 Bab Ezzouar, Alger, Algeria*

kahinabak@yahoo.fr

Abstract:

Vitamin E is a very important compound of biological membranes, due to its multiple roles. Several studies suggest that vitamin E may contribute to help lower the risks of specific chronic and degenerative diseases such as alzheimer, age-related macular degeneration, some types of cancer, cataracts and ischemic heart disease. Herein the vanadyl (II) was connected with two vitamin E and two water molecules. Our studies performed at a purely theoretical level, show structural and spectroscopic properties of the complex VO (Vit E)₂(H₂O)₂ that is known as a good agent to treat diabetes.

This large system implies the use of an ONIOM (QM/MM) method. The QM part was treated by DFT/PBE0/6-31+g(d), whereas the UFF method was used to study the second part. The obtained results were compared to available experimental data.

Key words: anti-diabetic effect, complex of vitamin E, ONIOM method, structural and spectroscopic properties.

PO 10

Study of MIM structures for HF detection

R. Becharef, K. Saïl and G.Bassou

L2MSM laboratory - Faculty of Exact Sciences Djilali Liabes University. 22000. Sidi Bel-Abbes. Algeria

rbecharef@yahoo.fr

Abstract:

The MIM (metal insulator metal) structures can be used as capacity, memory, frequency mixer or detector. These functions depend largely on the oxide. In this work, we have realized and characterized MIM structures. We used aluminum in the bottom, its oxide in the middle that will play the role of insulation and the upper metal we used gold that we obtained by spraying. The characteristics thus obtained show that these structures can be used as good sensors with high frequencies (HF).

Keywords: MIM diodes, detectors, Schottky Diodes



PO 11

Comparative Morphology, Structure and Optical Properties of Al, Cu and Sn Doped ZnO Nanostructure Synthesized by Spray Pyrolysis

A. Bedia*, F. Z. Bedia*, M. Aillerie**, N. Maloufi*** and B. Benyoucef*

* *URMER, Abou-Bakr Belkaid University - Tlemcen, Algeria*

asma.bedia@mail.univ-tlemcen.dz

f_bedia@yahoo.fr

benyoucef_boumediene@yahoo.fr

** *LMOPS-EA 4423, Université de Lorraine - METZ, France / LMOPS, Supelec - Metz, France*

aillerie@metz.supelec.fr

*** *Laboratoire d'Étude des Microstructures et de Mécanique des Matériaux (LEM3), UMR CNRS 7239, Université de Lorraine - Metz, France / Laboratory of Excellence on Design of Alloy Metals for low-mAss Structures (DAMAS), Université de Lorraine - Metz, France*

nabila.maloufi@univ-lorraine.fr

Abstract:

The effects of different dopants (Cu, Al, Sn) on the morphology, structure and optical properties of ZnO thin films synthesized by chemical spray pyrolysis technique on glass substrates have been investigated by thermal field emission gun scanning electron microscope (FESEM), X-ray diffraction technique (XRD) and optical characterization method. FESEM images of ZnO:Cu, ZnO:Sn and ZnO:Al thin films show that the surface morphology is strongly affected by the nature of the doping element. All films are polycrystalline with a structure that belongs to the hexagonal Wurtzite type. The high diffraction intensity of the (0002) peaks for ZnO:Sn and ZnO:Al indicates that these films exhibit a relatively preferential orientation with c-axis perpendicular to the surface, except ZnO:Cu thin film exhibits a (10 $\bar{1}$ 1) preferred orientation. The lattice parameters change slightly with doping. All samples exhibit a high transmission in the visible range ($> 70\%$). The optical bandgap E_g and the Urbach energy EU change with doping. As the optical properties also depend strongly on doping, this doping strategy remains the key for optimized films as function of various intended applications.

Key words: ZnO nanostructures, spray pyrolysis, doping effects, XRD, FESEM, optical properties.



PO 12

Growth and Characterization of Tin Doped ZnO Thin Films

F. Z. Bedia*, A. Bedia*, M. Aillerie**, N. Maloufi*** and B. Benyoucef*

* URMER, Abou-Bakr Belkaid University - Tlemcen, Algeria

f_bedia@yahoo.fr

asma.bedia@mail.univ-tlemcen.dz

benyoucef_boumediene@yahoo.fr

** LMOPS-EA 4423, Université de Lorraine - METZ, France / LMOPS, Supelec - Metz, France

aillerie@metz.supelec.fr

*** Laboratoire d'Étude des Microstructures et de Mécanique des Matériaux (LEM3), UMR CNRS 7239, Université de Lorraine - Metz, France / Laboratory of Excellence on Design of Alloy Metals for low-mAss Structures (DAMAS), Université de Lorraine - Metz, France

nabila.maloufi@univ-lorraine.fr

Abstract:

Sn-doped Zinc Oxide (ZnO:Sn) films have been deposited by spray pyrolysis method on glass substrate, where the Sn/Zn atomic ratio was (0, 0.5, 1, 1.5 and 2%) in the solution. The effects of Sn incorporation on morphological, structural and optical properties of ZnO films were investigated. High resolution Field Effect Scanning Electron Microscopy characterization showed that the films consist of hexagonal-like grains and the morphological surface was affected by Sn low doping. The X-Ray Diffraction (XRD) patterns showed that all films have polycrystalline structures, and the doping incorporation has not lead to substantial changes in the structural characteristics of ZnO films. The measurements from UV-Visible Spectrophotometer (U-Vis) indicated that all films are highly transparent (73–93%) in the visible region. The effect of Sn content on the optical band gap and Urbach energy values was studied. A blue shift of the optical band gap, attributed to the Burstein Moss effect, was observed for the Sn-doped films.

Key words: ZnO Films, Sn Doping, SEM Micrographs, X-Rays Patterns, Optical Properties



PO 13

THEORETICAL STUDY OF 3D TRANSITION METAL/GERMANIUM COMPOUNDS

A. Bekhti-Siad*, H. Riane*, M. B. Siad**, A. Mokrani***

**Laboratoire de Matériaux, Applications et Environnement LMAE, Faculté des Sciences et Technologies, Département de Sciences de la Matière, Université de Mascara, Route de Mamounia BP 29000 Mascara, Algérie*

siadmail@hotmail.com

riane_h@yahoo.fr

***Université de Mascara, Route de Mamounia BP 29000 Mascara, Algérie*

siad_benamar@yahoo.fr

****IMN, 2, rue de la Houssinière, BP 32229, 44322 Nantes, France*

Arezki.Mokrani@cnrs-imn.fr

Abstract:

We present a theoretical study of the electronic and magnetic properties of binary Ge and transition metal (TM) compounds and their TM mixed crystals having the C16 tetragonal structure as found in Al_2Cu . Ab initio calculations based on density functional theory were performed using a supercell containing 4 TM and 8 Ge atoms. For the compounds containing only a single kind of TM, FeGe_2 presents an antiferromagnetic configuration, MnGe_2 is ferromagnetic but CoGe_2 and CrGe_2 are both nonmagnetic. For the compounds with two different types of TM atoms, the magnetic order depends strongly on the relative position of the chemically different TM atoms. Moreover, in ultra thin film perpendicular to the tetragonal axis, both kinds of the former materials either pure or mixed, display magnetic properties though different from those of the corresponding bulk material. In all cases investigated the local magnetic moments increase when the top layer is of TM type.

Key words: Transition Metal, Ultra Thin Film, Bulk Material, Ferromagnetic and Antiferromagnetic order.

PO 14

Application of docking methodologies for the discovery of novel tumor cell migration inhibitors

Bekhti-Bensalem.N*, Pérez-Sánchez H** and Sekkal-Rahal.M*

*L2MSM laboratory - Faculty of Exact Sciences Djilali Liabes University. 22000. Sidi Bel-Abbes. Algeria

nabilachimie@yahoo.fr

majsekkal@msn.com

**Bioinformatics and High Performance Computing Research Group

Computer Science Department, Universidad Católica San Antonio de Murcia (UCAM), Spain

hperez@ucam.edu

Abstract:

Tumor metastasis is the primary cause of death of cancer patients. Development of new therapeutics preventing tumor metastasis is urgently needed. Migrastatin, which is a strong inhibitor of tumor cell migration, has been an important lead in the development of antimetastatic agents. The challenge is to show that it is very urgent to discover new analogs of Migrastatin targeting the actin-bundling protein fascin to inhibit its activity, and also other novel inhibitors with new scaffolds. These new compounds must show high values of binding affinity against fascin. For the prediction of binding affinities we used several docking techniques such as Autodock Vina.

Migrastatin, iso-migrastatin and lactimidomycin are all glutarimide-containing polyketides known for their unique structures and cytotoxic activities against human cancer cell lines. In this work we also study the interactions of iso-migrastatin and lactimidomycin and calculate the theoretical values for the affinity between fascin and related chemical analogs. Afterwards we perform a search for analogs using the ZINC database, which contains information about millions of compounds.

Key words: AutodockVina, ZINC Database, Fascin, iso-migrastatin, lactimidomycin, Migrastatin.



PO 15

Conformational characteristics of alginates and their interaction with the sodium ions: study by DFT

L. Bekri and M. Sekkal-Rahal

L2MSM laboratory. Faculty of Science. Djillali Liabes University of Sidi-Bel-Abbes, 22000.Algeria

Lahcene_bekri@yahoo.fr

Abstract:

The conformational analysis of the disaccharides composed of two units of alginic acid (β -D-mannuronic and α -L-guluronic acid) was performed using the functional theory of density at B3LYP/6-31G*level. The study covered disaccharides anionic, neutral salts of the acids such as sodium in an isolated state and in aqueous solutions using the PCM model approach. We analyzed the interactions of intramolecular hydrogen bond characterizing the lowest energy conformer. The results indicate that the values of the glycosidic dihedral angles may vary in the same way, irrespective of the composition of disaccharides. The presence of hydrogen bonds involving inter-residue carboxylic groups reduced binding capacity for calcium ion. The main effect of the formation of protonated and salt form on the distribution of electron density is limited to/formed near the carboxylate group environments broken interactions.

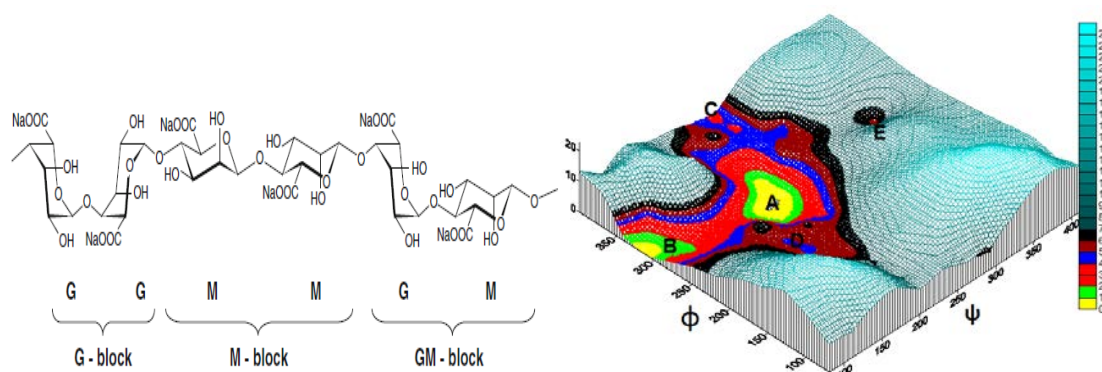


Fig.1 Relaxed iso-potential maps at the B3LYP/6-31G(d) level of compound MM in the gas phase. (ΔE in kcal/mol)

Key words: Alginate, DFT calculations, Conformation, Liaison hydrogen.

PO 16

Modeling of the electrical parameters of a dye-sensitized solar cell

M. Belarbi, A. Benyoucef, B. Benyoucef and Z.bouzid

*Research Unit Materials and Renewable Energy, Department of Physics University of Abou Bekr Belkaid-
Tlemcen, BP: 119 Tlemcen 13000, Algeria.*

b.moussaab@outlook.fr

abdellah.benyoucef@mail.univ-tlemcen.dz

boumediene.benyoucef@mail.univ-tlemcen.dz

bzd.zakaria@gmail.com

Abstract:

The dye-sensitized solar cells (DSSC) have gained in recent decades an important place among solar technologies due to their low cost of implementation and performance becomes more efficient. The experimental data for this type of cells are enriched and accumulated quickly, given the enthusiasm for this new technology. The present work is to present a model that links the electrical material parameters to cell performance; the cell is modeled as a "pseudo-homogeneous effective medium" consisting of a semiconductor of nanoporous TiO_2 , of light absorbing dyes and electrolyte. The macroscopic electric field, resulting in an unbalanced distribution of charge carriers under illumination, will be calculated with the Poisson equation. The front and rear limits of the cell will be modeled as a metal-semiconductor ohmic contact and as a redox electrode via the voltage-current equation, respectively. The limitations of this model are discussed and compared with some experimental data from the literature, and providing opportunities to improve the model.

Key words: DSSC, TiO_2 , An electrical model, I - V Characteristics.

PO 17

Estimation of the Acute Toxicity of Halogenated Phenols using Semi-empirical Quantum Chemistry Methods

Khadidja Bellifa* and Sidi Mohamed Mekelleche**

**Laboratory of Applied Thermodynamics and Molecular Modeling, Department of Chemistry, Faculty of Science, University of Tlemcen, BP 119, Tlemcen, 13000, Algeria*

kbellifa@yahoo.com, k_bellifa@mail.univ-tlemcen.dz

***Preparing School in Sciences and Techniques of Tlemcen, BP 165 RP Bel Horizon, 13000, Tlemcen, Algeria*

sm_mekelleche@mail.univ-tlemcen.dz

Abstract:

Phenols and especially halogenated phenols represent a substantial part of the chemicals produced worldwide and are known as aquatic pollutants. Quantitative structure–activity relationship (QSAR) models are useful in understanding how chemical structure relates to the toxicity of chemicals. In the present study, the acute toxicity of 45 halogenated phenols was analysed using no consuming time and cost semi empirical AM1, PM3, and PM6 methods to calculate quantum chemical descriptors. QSAR models were developed using multiple linear regression technique. The predictive ability of the models was evaluated by the internal cross validation, the Y-randomization technique and the external validation. Their structural chemical domain has been verified by the leverage approach. The statistical results obtained with the AM1 method indicated that the multiple correlation coefficient (R^2) and cross validation using leave-one-out (R^2_{cv}) are 0.91, 0.90 respectively. While the external validation gave (R^2_{ext}) about 0.96. These showed that the developed QSARs models using a small number of descriptors interpretable have good stability, robustness and high predictive power. The developed QSAR models clearly show the importance of the semi-empirical methods to calculate the electrophilicity indices in ecotoxicological studies.

Key words: Toxicity mechanism, halogenated phenols, Parr's electrophilicity index, semi-empirical method, hydrophobicity.



PO 18

Structural and mechanical properties of YM₂ (M: Ni, Cu, Zn) Laves phases studied by first-principles calculations

M.K. Benabadji* and H.I. Faraoun**

* *Laboratoire d'Etude et Prédiction des Matériaux, Unité de Recherche Matériaux et Energies Renouvelables, LEPM-URMER, Université de Tlemcen, Algeria*
kbenabadji@yahoo.fr

** *Laboratoire d'Etude et Prédiction des Matériaux, Unité de Recherche Matériaux et Energies Renouvelables, LEPM-URMER, Université de Tlemcen, Algeria*
faraoun@atrst.dz

Abstract:

Ab initio calculations have been performed to calculate the density of states (DOS), charge density distribution and enthalpy of formation of main YNi₂, YCu₂ and YZn₂ binary Laves phases with C14, C15, C36 and CeCu₂ in Ni-Cu-Y-Zn alloy are investigated by first-principles calculations with a stacking of atomic chain to reveal its electronic structure. The results show a covalent bonding between Ni-Ni, Cu-Cu, Zn-Zn, a metallic bonding between Y-Y in YM₂ (M: Ni, Cu, Zn) and polar covalent bonding between Y-M. Differences in the mechanical properties can be explained by the calculated bonding characteristics. Density functional theory is considered within framework of both pseudo-potentials and plane waves basis using VASP (Vienna ab initio Software Package).

Key words: Ab initio calculations DFT, Laves phases, Intermetallics, Structural and mechanical properties, CeCu₂ orthorhombic structure.

PO 19

Structural study of Sodium Lauryl Ether Sulfate and Sodium dodecyl sulfate by molecular modeling

Abdellatif Benahmed and Zizi Zahia

*Laboratory of Materials and Catalysis, Chemistry Department, Faculty of Sciences, Hailarbi Ben M'hidi BP
89 University of Sidi- Bel- Abbès; SIDI BEL ABBES, 22000, Algeria*

Abdellatif.Benahmed @ yahoo.fr

z_zahia@yahoo.com

Abstract

The detergent industry mainly uses surfactants which are deposited on land and into water systems. Some of them are known to be toxic to animals, ecosystems, and humans, and can increase the diffusion of other environmental contaminants. Indeed, their presence in water, even in small amounts, changes its flavor, color and odor making it unfit for consumption or toxic.

In recent years computer tools allowed the chemistry to make a further study to understand the behavior of molecular systems using molecular modeling

In this work, we studied the structure of two anionic surfactants, Sodium Lauryl Ether Sulfate $\text{CH}_3 (\text{CH}_2)_{11}(\text{OCH}_2\text{CH}_2)_3\text{OSO}_3\text{Na}$ and Sodium dodecyl sulfate $\text{CH}_3 (\text{CH}_2)_{11}\text{OSO}_3\text{Na}$ by molecular modeling. First we performed molecular mechanics calculations, to optimize the geometry and minimize energy. In a second time, we calculated the sizes of the two pollutants to explore the possibilities of their adsorption on five types of montmorillonite (Mt (natural), Mt (Na), Mt (Ca), Mt (K) and Mt (Mg)).

The results of our calculations showed that Sodium Lauryl Ether Sulfate and Sodium dodecyl sulfate adsorb on Mt (natural), Mt (Ca) and Mt (Mg). While on Mt (Na) and Mt (K), the two anionic surfactants can't be adsorbed.

Key words: Adsorption, Clay, Molecular mechanics, Molecular modeling, Montmorillonite, Surfactants.

PO 20

Study of structural, elastic and electronic properties of TbX (X=N, P, As, Sb) compounds using LSDA and LSDA+U approach.

B. Benbahi*, H. Bouafia*, A. Akriche*, N. Benkhattou**, S. Hiadsi*, D. Rached** and B. Abidri**

*Laboratoire de Microscope Electronique & Sciences des Matériaux USTO, département de physique, BP1505 El m'naouar, Oran, Algérie.

**Laboratoire des matériaux magnétiques Université Djillali Liabbès 22000 Sidi Bel-Abbès, Algérie

Abstract:

Structural, elastic and electronic properties in the cubic TbX(X=N, P, As, Sb) compounds are derived from the full-potential linear muffin-tin orbital method, within the frame of density functional theory (DFT). The exchange correlation energy is described in the local spin density approximation LSDA, using the Perdew-Wang parameterization. The equilibrium lattice parameters, bulk modulus, transition pressure, elastic constants and their related parameters such as Poisson's ratio, Young modulus, shear modulus and Debye temperature were calculated. We compared our obtained results with available experimental and theoretical data. They are in reasonable agreement. The electronic properties are treated also with LSDA+U approach. Our results show that both compounds exhibit half metallic behaviour.

Key words: FP-LMTO, LSDA+u, ground state, elastic constants, electronic properties,



PO 21

Regio- and Diastereoselectivity of the 1,3-Dipolar Cycloaddition of α -aryl Nitron with Methacrolein. A

Theoretical Investigation

Wafaa Benchouk* and Sidi Mohamed Mekelleche**

*Laboratory of Applied Thermodynamics and Molecular Modelling, Department of Chemistry, Faculty of Science, University of Tlemcen, PB 119, Tlemcen, 13000, Algeria

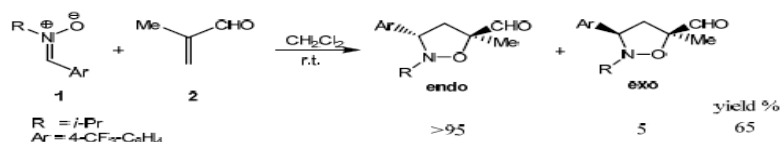
Wafaab2@yahoo.fr

**Preparing School in Sciences and Techniques of Tlemcen, BP 165 RP Bel Horizon, 13000, Tlemcen, Algeria

sm_mekelleche@mail.univ-tlemcen.dz

Abstract:

The mechanism, regio- and diastereoselectivity of the 1,3-dipolar cycloaddition of N-isopropyl, α -(4-trifluoromethyl)-phenyl nitron with methacrolein yielding the isoxazolidine cycloadduct has been studied at the B3LYP/6-31G(d) level of theory (see Scheme1). All the possible regio- (meta/ortho) and stereo- (endo/exo) isomeric channels to provide the different diastereoisomers were thoroughly investigated. The free activation enthalpies, calculated with the MPW1B95/6-31G(d) method, in dichloromethane show that the meta-endo cyclisation mode giving the (RR, SS) couple of diastereoisomers is the most favoured reaction channel as expected experimentally. Intrinsic reaction coordinate (IRC) calculations and the topological analysis of the electron localization function (ELF) of some relevant points of the IRC curve show that the meta-endo favoured channel takes place via a one-step two-stage mechanism and the formation of the two new sigma bonds is highly asynchronous. Charge transfer calculations performed at the transition states in combination with the calculation of DFT-based reactivity indices of the reactants indicate a low polar character of the studied reaction.



Keywords: 1,3-Dipolar Cycloaddition, Nitron, Isoxazolidine, Regioselectivity, Diastereoselectivity, Density functional theory.

PO 22

Electronic and mechanical properties of the fluoroperovskite LiBeF_3

M. Benkabou, Kourdassi, N. Benkhetrou and D. Rached

Laboratoire des matériaux magnétiques Université Djillali Liabbès 22000 Sidi Bel-Abbès, Algérie

Abstract:

First-principles calculations have been used to investigate the structural, electronic and elastic properties of LiBeF_3 in perovskite structure, using the full-potential linear muffin-tin orbital (FP-LMTO) method. The exchange correlation energy is described in the local density approximation (LDA) using the Perdew–Wang parameterization. The results of the electronic properties show that this compound is an indirect band gap material which is in good agrees with experimental results. A special interest has been made for the determination of the elastic constants, Electron effective mass, hole effective mass parameters and The energy band gaps and their volume and pressure dependence are investigated which have not been established experimentally or theoretically.

Keywords: ab-initio calculations; Electronic structure; transport properties; Elastic constants.

PO 23

Theoretical study and Born Oppenheimer Molecular Dynamics calculation of the ν O-H IR Spectra for Acetic Acid Cyclic Dimers

Mohamed El Amine Benmalti*, Marie-Pierre Gageot** and Krallafa Abdelghani***

*: *aLaboratoire de Structure Elaboration et Application des Matériaux Moléculaires, Université Abdelhamid Ibn Badis Mostaganem, 27000, Algeria*

** : *LAMBE Laboratoire Analyse et Modélisation pour la Biologie et l'Environnement Blvd François Mitterrand – Bat Maupertuis - 91025 EVRY Cedex – France*

***: *Laboratoire de Chimie Physique Macromoléculaire, Université d'Oran (Es Senia) Oran 31000*

malti23@yahoo.fr

Abstract:

Both ab initio molecular dynamics simulations based on the Born-Oppenheimer approach calculations and a quantum theoretical model are used in order to study the IR spectrum of the acetic acid dimer and its deuterated in the gas phase. The theoretical model is taking into account the strong anharmonic coupling, Davydov coupling, multiple Fermi resonances between the first harmonics of some bending modes and the first excited state of the symmetric combination of the two ν O-H modes and the quantum direct and indirect relaxation. The IR spectra obtained from DFT-based molecular dynamics is compared with our theoretical lineshape. Note that in a previous work we have shown that our approach reproduces satisfactorily the main features of the IR experimental lineshapes of the acetic acid dimer¹.

Key words: H-bond, Fermi resonance, Strong anharmonic coupling theory, Infrared spectra, Linear response theory, Indirect and direct relaxation, Davydov coupling.

References:

Theoretical interpretation of the infrared lineshape of liquid and gaseous acetic acid” Mohamed el Amine Benmalti, Paul Blaise, H. T. Flakus, Olivier Henri-Rousseau, Chem Phys, 2006 vol 320, 267-274



PO 24

Discretization of continuum states. Application to the atomic excitation

N.E. Houda. Benmansour*, M. Bouamoud** and Mohammed Sahlaoui***

*Abou Bekr Belkaid University, Tlemcen, Algeria.

nour_mansour1@yahoo.fr

**Naama University Centre, Algeria.

m_bouamoud@yahoo.fr

***Preparatory School in Science and Technology, Tlemcen, Algeria.

mohammed.sahlaoui@gmail.com

Abstract:

We have developed a variational method based on the variational principle of Schwinger, to apply it to the excitation of atoms by ion impact in the energy range excluding a processing disruption. To describe the strong coupling between the excitation pathways and capture that exists at low energy we introduced the continuum states in the total wave function of diffusion. We present a method for calculating analytical elements of discrete-continuous and continuous - continuous involved in the transition amplitude matrix.

Keywords: Transition amplitude, Schwinger variational principle, atomic collisions, the continuum states.



PO 25

Polymer based photovoltaic solar cells: Prospects and challenges

Amel Benmouna, Réda Benmouna and Boumédiène Benyoucef

URMER, Faculty of sciences, University of Tlemcen PB 119 Algeria

Amel.benmouna@yahoo.fr

benyoucef_boumediene@yahoo.fr

redabenmouna@email.com

Abstract:

Since Shirakawa, McDermid and Heeger (Nobel laureates of chemistry in 1990) have demonstrated in the seventies that conjugated polymers can be used as semiconductors, there has been a tremendous effort to develop polymer based photovoltaic solar cells. These pionners focused on the conductive properties of polyacetylene (CH)_x but since their discovery, a wide variety of polymers has been covered changing not only the monomer species but considering also different chain architectures and other novel species such as fullerene, carbone nanotubes, quantum dots and their derivatives. Polymers offer great advantages over inorganic semiconductors such as the availability of a large number of species at relatively low cost, eas in synthesis, the possibility of developing large surface panels and a much higher flexibility. The main drawback at present time is the insufficient overall efficiency which remains near 10% compared to silicium based cells that enable much higher efficiencies. The purpose of this communication is to demonstrate that this situation can be changed and conjugated polymers can lead to improved efficiencies making them a real alternative to silicium for a clean renewable energy source. We review the successive steps in the process of transformation of solar radiation to electrical current pointing out the aspects where research can lead to possible brackthroughs along these lines.

Key words: Conjugated polymers, semiconductors, solar cells, photovoltaic, efficiency.

PO 26

Electric and dielectric studies of the $[\text{N}(\text{CH}_3)_3\text{H}]_2\text{CuCl}_4$ compound at low temperature

A. Ben Rhaïem*, M. Ben Bechir*, K. Karoui*, A. Bulou** and K. Guidara*

*: University of Sfax, Faculty of Sciences, Laboratory of Condensed Matter, BP1171, 3018 Sfax, Tunisia

abdallahrhaïem@yahoo.fr

mohamedbenbechir@hotmail.fr

karouikimi@yahoo.fr

kamelguidara@yahoo.fr

** : LUNAM Université, Université du Maine, CNRS UMR 6283, Institut des Molécules et Matériaux du Mans (IMMM), Avenue Olivier Messiaen, F-72085, Le Mans Cedex 09, France

Alain.Bulou@univ-lemans.fr

Abstract:

The $[\text{N}(\text{CH}_3)_3\text{H}]_2\text{CuCl}_4$ compound is obtained by slow evaporation at room temperature and it is characterized by XRD which shows that this compound crystallizes in the monoclinic system with $\text{P2}_1/\text{c}$ space group. Four phase transitions at low temperature are found by differential scanning calorimetric. The material is characterized by impedance spectroscopy technique measured in the 10^{-1} - 10^6 Hz frequency and 203-313K temperature ranges. The dielectric permittivity indicates a ferroelectric–paraelectric phase transition at 293K. Analysis of Nyquist plots revealed the contribution of three electrically active regions corresponding to bulk mechanism, distribution of grain boundaries and electrode processes. The modulus plots are characterized by the presence of two peaks associated with the grain and the grain boundaries. The temperature dependence of the electrical conductivity (σ_g) and AC conductivity (σ_{ac}) confirms the phase transitions at $T_1=226\text{K}$, $T_2=264\text{K}$, $T_3=297\text{K}$.

Keywords: Ferroelectric, Complex impedance, Dielectric Modulus, AC conductivity.

PO 27

Theoretical study of the clusters $(\text{ZnO})_6$ substituted by tellurium atoms

Nour el Houda. Bensiradj* and Ourida .Ouamerali*

**Laboratory of theoretical Chemistry Computational and Photonic (LCTCP)*

Faculty of chemistry, USTHB, PC: 16111 El Al alia, Algiers, Algeria

nourelhouda.bensiradj@yahoo.fr

ouameralio@hotmail.fr

Abstract:

The nano structures of ZnO had attracted much interest due to its wide range of applications, which include optoelectronics, glass industries and solar cells. These compounds have a great advisability of creating new materials employed in energy technologies.

In this work we studied a series of nano structures $(\text{ZnO})_6$ by using the technique of doping, we introduce impurities on the level of the geometry of these clusters, by replacing each time an oxygen atom by a tellurium atom.

The clusters obtained (containing tellurium atoms) show interesting characteristics in the system development at solar energy. The calculation of geometric parameters of the ground state of $(\text{ZnO})_6$ nanoclusters with telluride applied as substitutional Impurity at different locations within the structure was carried out using Density Functional Theory (DFT) approach with the B3LYP level and LANL2DZ basis set. Excited state energies, as well as absorption wavelength, were calculated using Time Dependent-Density Functional Theory (TDDFT). For the emission wavelength, the excited state geometry optimization was obtained with Hartree – Fock Configuration Interaction Singles (HF/CIS). Our work led us to significant results; that the clusters studied were employed in the detection of the radiation terahertz (THZ), which could replace x-rays for the applications in radiology. These clusters are also used in the system development to solar energy as well as the manufacture of electroluminescent diodes (LED) emitting in the visible area of the electromagnetic spectrum.

Key words: The clusters $(\text{ZnO})_6$, tellurium, DFT, TDDFT.



PO 28

DFT AND MP2 CONFORMATIONAL STUDY OF 3, 6 ANHYDRO- α -D-GALACTOSE MOLECULE IN GAS PHASE AND IN WATER

N. Bestaoui-Berrekchi-Berrahma*, M. Rahal-Sekkal* and N. Yousfi*

*Faculté des Sciences, Laboratoire L2MSM, Université Djillali Liabes de Sidi Bel Abbès,
B.P.89, Sidi Bel Abbès, 22000, ALGERIA

noreya.bestoui@gmail.com

majsekkal@msn.com

nordyp@gmail.com

Abstract:

Density functional and MP2 calculations have been carried out on 3,6-anhydro- α -D-galactose, one of the monosaccharides constituting carrageenans. Carrageenan structures are based on linear chains of alternating 3-linked β -D-galactopyranosyl units, and 4-linked α -D-galactopyranosyl (or 3,6-anhydro- α -D-galactopyranosyl) units, usually sulfated in different positions. The molecular flexibility, is concentrated mostly on the glycosidic linkages.



Figure1 : Structures of 3,6-anhydro- α -D-galactose.

In this study, we examined the structure and the energy of the monosaccharide 3,6 anhydro- α -D-galactose constituting neocarrabiose (3-O-(3,6-Anhydro- α -D-galactopyranosyl)- β -D-galactopyranose or β -D-neocarrabiose) (fig.1). DFT calculations using the B3LYP/6-31G(d) basis set were carried out on different conformers of the molecule. Relaxed iso-potential maps, show where regions of low energy occur in the dihedral angles: (χ_2 , χ_1), (χ_4 , χ_1) and (χ_4 , χ_2) for monosaccharide. These energetic contour maps, performed in the gas phase (fig.2) and then in aqueous medium using two models to simulate the solvent effect; the Onsager and the polarized continuum (PCM) models, have been built as suggested by French and Dowd by interpolating a set of data comprising a total of 324 energy values for monosaccharide. Once the set of the two

specific values of dihedral angles fixed (χ_2, χ_1), (χ_4, χ_1) and (χ_4, χ_2) for monosaccharide, they were kept frozen while optimizing all of the other geometrical parameters. The lower energy conformers were then fully optimized using B3LYP, B3PW91 and MP2 functionals with several basis sets.

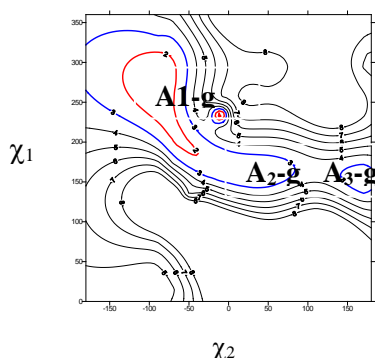


Figure 2: Relaxed iso-potential maps at the B3LYP/6-31G(d) level of 3,6-anhydro- α -D-galactose (χ_2, χ_1) in gas phase. (ΔE in kcal/mol).

Table 1: χ_1 and χ_2 (in degrees) and relative energies (Kcal/mol) at the B3LYP/6-31G(d) level in gas phase and in water for 3,6-anhydro- α -D-galactose (χ_2, χ_1) .

Conformer	Gas phase		Water: Onsager		Water: PCM		Conformer		
	ΔE	χ_2, χ_1	Conformer	ΔE	χ_2, χ_1	Conformer	ΔE	χ_2, χ_1	
A1-g	0.00	-90, -105	A1-On	0.00	-92, -81	A1-PC	0.00	1, 155	
A2-g	0.76	30, 154	A2-On	0.51	28, 159	A2-PC	1.80	-39, -25	
A3-g	0.79	170, 154	A3-On	1.45	168, 159	A3-PC	3.10	-39, 15	

The two energetic maps related to (χ_2, χ_1) in the gas phase and in implicit solvent with Onsager model are very similar. This fact confirms the limitation of Onsager model as pointed out in a previous paper despite the fact that the considered monosaccharide has a shape which can be easily introduced into as a spherical cavity as in the Onsager model. The PCM model provides three different minima of the gas phase.

Key words: 3,6-anhydro- α -D-galactose, Relaxed iso-energetic maps, DFT methods, Gas phase, solvent, Polarizable continuum model, Quantum mechanics methods.

PO 29

Structural, electronic, and magnetic properties of RbSrX(C, Si, Ge) half-Heusler

A. Bouabça*, A. Amar*, and H. Rozale*

**Condensed Matter and sustainable development Laboratory (LMCDD), University of Sidi Bel-Abbès, Sidi Bel-Abbès 22000, Algeria.*

bouab.asma@yahoo.fr

a.ama@yahoo.fr

hrozale@hotmail.fr

Abstract:

Electronic structure and magnetic properties based on density functional theory (DFT) within the generalized gradient approximation (GGA) for RbSrX(X= C, Si, Ge) half-Heusler compounds have been performed using the full-potential linearized augmented plane wave (FP-LAPW+lo) method. The electronic band structures and density of states of three compounds show that the spin-down electrons have metallic, and the spin-up bands have a gap of 1.73, 1.61, and 1.23 eV for RbSrC, RbSrSi, and RbSrGe respectively, resulting in stable half-metallic ferromagnetic behavior with magnetic moments of 1 μ_B .

Key words: half-Heusler compounds; half-metallic ferromagnetic; FP-LAPW+lo.



PO 30

Bioconcentration factor of PolyChloroBiphenyl in the environment: modeling and QSPR study

N.Bouarra*, H.Boufenaya*, H.Haddag* and D.Messadi*

* *Laboratoire de Sécurité Environnementale et Alimentaire (LASEA)/ Université BADJI Mokhtar- Annaba.*

Faculté des sciences. Département de chimie.

b_nabil@voila.fr

Hamza_Boufenaya@yahoo.fr

haddaghamza@yahoo.fr

d.messadi@voila.fr

Abstract:

The Polychlorinated biphenyls, or PCBs, are chlorinated chemical derivatives. These compounds are widely used in industry for their electrical insulation, flame resistance and lubrication qualities. They were found particularly as insulators in electrical transformers, as lubricants or as oils components or of welds. PCBs are poorly biodegradable and have physicochemical properties that confer a high potential for bioaccumulation in organisms; they are still very much at present in aquatic ecosystems. The issue of contamination of aquatic ecosystems and the potential impact on human health arises more and more. It is important to understand the presence and fate of PCBs in the environment deepen understanding of the sources themselves, but also to study the mechanisms of dispersion, processing and transport. An important molecular property such as the bioconcentration factor plays a fundamental role in the behavior of PCBs. Knowledge of BCF is necessary for predicting the environmental fate of PCBs, BCF values of many compounds are not available in the literature, their measure is costly and time consuming, the QSPR methods are becoming a necessity for it in this study, we constructed a QSPR model, which will help us to predict the value of the BCF; we applied the method of multiple regression to link BCF to the molecular structures, the selection of descriptors was made by genetic algorithm. The results obtained show that the model is very robust and its predictive ability is important $Q^2_{LOO} = 86.87 \%$, $R^2 = 91.89 \%$, $Q^2_{EXT} = 87.88 \%$ in addition to the model is highly significant $F = 59.52$.

Key words: ecosystem, environment, semiempirical, PM3, QSPR, BCF, MLR.

PO 31

Influence of the used solvation model on the computation of electronic spectra of metal complexes: the example of Al(III)-caffeic acid system

Sonia Boumendil^{*/**}, Aurélien Moncomble^{*}, Jean-Paul Cornard^{*} and Majda Sekkal-Rahal^{**}

**LASIR, CNRS UMR 8516, Université des Sciences et Technologies de Lille, Bât. C5,
59655 Villeneuve d'Ascq Cedex, France*

Sonia.Boumendil@univ-lille1.fr ,

aurelien.moncomble@univ-lille1.fr

Jean-Paul.Cornard@univ-lille1.fr

*** Laboratoire de Microscopie, Microanalyse de la matière et Spectroscopie Moléculaire,
Université Djilali Liabès, B.P 89, Sidi Bel Abbès 22000, Algérie.*

majdasekkal63@gmail.com

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. 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.

PO 32

Ab initio analysis of the conformations of Acetylcholine

A. Boutasta and A. Benosman

Laboratoire Physique Théorique -B.P 119 Chetouane 13000 Tlemcen, Algérie.

aboutasta@gmail.com

h_benos@yahoo.fr

Abstract:

The conformational properties of acetylcholine have been the subject of a greater number of theoretical investigations than have been those of any other molecule of pharmacological interest.

The potential energy surfaces of acetylcholine were obtained and plotted in terms of energy versus the two central dihedral angles of the molecule.

Key words: Acetylcholine; Conformational analysis; DFT; Ramachandran map.

PO 33

Estimation of solar radiation and sizing method for autonomous photovoltaic system. Application to the west of Algeria

Z.Bouzid, N.Ghellai and M. Belarbi

Research Unit Materials and Renewable Energy, Department of Physics University of Abou Bekr Belkaid-Tlemcen, BP: 119 Tlemcen 13000, Algeria

bzd.zakaria@gmail.com

na_ghellai@yahoo.fr

b.moussaab@outlook.fr

Abstract:

The Algeria, a North African country, have a large quantity of solar energy (first in the Mediterranean sea). This deposit makes it suitable for the implementation of solar energy conversion systems, particularly photovoltaic (PV) systems. The design of these systems is an important step, its optimization, as well as the optimization of different parameters, is a crucial operation. In our work, after estimating hourly solar radiation, we optimized the design of an autonomous photovoltaic system at “Zenata” (Tlemcen), west of Algeria, by focusing on the efficiency of the PV panels, the total collecting area and the battery capacity.

We relied on the concept of solar utilizability to develop a design method that contains several steps.

Key words: Photovoltaic, utilizability, design, optimization, hourly solar radiation, Algeria.



PO 34

A DFT Relativistic Study of Cyanide $[\text{MN}^*_3(\text{CN})_2]^{2-}$ and Isocyanide $[\text{MN}^*_3(\text{NC})_2]^{2-}$ ($\text{M}^{+3} = \text{Ce}, \text{U}$; $\text{N}^* = \text{N}(\text{SiMe}_3)_2$) Complexes.

Yamina Bouzidi*, Lotfi Belkhiri*, Abdou Boucekkine** and Michel Ephritikhine***

* *URCHEMS, Département de Chimie, Université de Constantine 1, 25000 Constantine, Algérie*

Yamina.bouzidi@gmail.com

lotfi.belkhiri@umc.edu.dz

** *Institut des Sciences Chimiques de Rennes, UMR 6226 CNRS-Université de Rennes 1, Campus de Beaulieu, 35042 Rennes Cedex, France*

abdou.boucekkine@univ-rennes1.fr

*** *CEA, IRAMIS, NIMBE, UMR 3299 CEA/CNRS SIS2M, CEA/Saclay, Bat 125, 91191 Gif-sur-Yvette, France*

michel.ephritikhine@cea.fr

Abstract:

The cyanide ion is one of the strongest ligands, with different ligation modes, and it is able to coordinate metal ions in their different oxidation states, affording a rich structural variety. In combination with the f elements, having strong Lewis acidity, large ionic radii, flexible coordination geometries and mainly polar metal–ligand interactions. For uranium, numerous oxidation states and unpaired f electrons, attractive compounds with novel physicochemical properties are expected to be obtained.

In this work we have performed a theoretical calculation on Cyanide $[\text{MN}^*_3(\text{CN})_2]^{2-}$ and Isocyanide $[\text{MN}^*_3(\text{NC})_2]^{2-}$ ($\text{M}^{+3} = \text{Ce}, \text{U}$; $\text{N}^* = \text{N}(\text{SiMe}_3)_2$) Complexes, which have been synthesized and X-ray characterized. All molecular geometries were fully optimized at relativistic DFT level of theory using the Amsterdam Density Functional (ADF2013.01) program package. Scalar relativistic effects were taken into account via the Zeroth Order Regular Approximation (ZORA). In order to provide a better understanding of the metal–ligand bonding, a Natural Population Analysis (NPA) and a Quantum Theory Atom-in-Molecules (QTAIM) analysis have been carried out. A good agreement was obtained between our results and the experimental available structural data.

Key words: Complexes f, Cyanide/isocyanide ligand, DFT/ZORA, Differentiation An(III)/Ln(III).

Reference:

Alexandre Hervé, Yamina Bouzidi, Jean-Claude Berthet, Lotfi Belkhiri, Pierre Thuéry, Abdou Boucekkine, and Michel Ephritikhine, *Inorg. Chem.*, **2014**, 53, 6995–7013



PO 35

Ab-initio calculations of the electronic structure and the magnetic properties of perovskite ruthenate CaRuO_3 : Good candidate for the fabrication of superconducting multilayers

Chahed Abbas, Rozale Habib, Hamdad Noura, Lakdja Abdelaziz and Benhelal Omar

Condensed Matter and Sustainable Development Laboratory, Physics Department

Djillali Liabès University of Sidi Bel-Abbès, Algeria.

omar_benhelal@yahoo.fr

Abstract:

We study the two pseudo-cubic perovskite ruthenate CaRuO_3 by means of LSDA electronic structure calculations using the FP-LAPW method for the real orthorhombic structure in para-, ferro-, and A-, C-, and G-type antiferromagnetic configurations. The LSDA calculations predict that orthorhombic structure are ferromagnetic, with total magnetic moments of 1, 9 μ_B . Our results are analyzed with the help of total, site-, spin-, and orbital-projected density of states. The general features of the DOS are in reasonable agreement with the experimental photoemission and other calculations. However, the fine details of the DOS of these structures are sharply peaked near the position of ϵ_F and this contributes to the high sensitivity of many of the calculated results as well as to strong variations of the properties of the real material. Our calculations show that the Ru d eg-like electrons are present in the whole valence-band region. Oxygen 2p-derived states hybridize strongly with Ru d states in this compound, and O, through this hybridization, plays an unusually large role in the magnetic properties. This involvement of O is responsible for the colossal magnetoresistance (CMR) coupling that is found in the calculations. Magnetic moments are examples of quantities exhibiting strong variations, but the calculations clearly show that the orthorhombic distortion is favourable for large spin splitting and low conductivity. A gap structure in the majority band just above ϵ_F can be important for semi-metallic properties induced by distortions or charge transfers.

Key words: Perovskite compound, Alkali metal, Ferromagnetism, Density functional theory.

PO 36

Theoretical Explanation of the Effect of 1-ethyl-pyridinium Trifluoroacetate Ionic Liquid in the Promotion of Diels–Alder Reactions of Isoprene with acrylic acid

Hafida Chemouri^{*/**}, Sidi Mohamed Mekelleche^{**}

**Laboratory of Applied Thermodynamics and Molecular Modeling, Department of Chemistry, Faculty of Science, University A. Belkaid, B. P. 119, Tlemcen, 13000, Algeria*

***Preparing School in Sciences and Techniques of Tlemcen, BP 165 RP Bel Horizon, 13000, Tlemcen, Algeria*

hafidachemmouri@yahoo.com

sm_mekelleche@mail.univ-tlemcen.dz

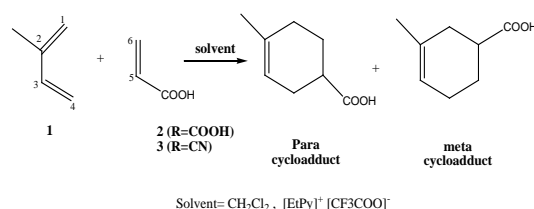
Abstract:

The design and discovery of Ionic Liquids (ILs) displaying melting point lower than 100 °C, in particular Room Temperature Ionic Liquids (RTILs) have been the subject of considerable efforts over the last decades. In particular, RTILs attract considerable attention because they are expected ideal solvents that provide novel reactions fields in the green chemistry. Recently, an increased attention has been focused on the development of green methods for the purpose of improving rate and selectivity of this reaction. This is mainly due to their favorable inherent properties such as chemical and thermal stability, no measurable vapor pressure, non toxicity, non flammability, catalytic ability, high polarity, ease to recycle, etc.

The Diels–Alder (DA) reaction is a powerful tool in organic synthesis and in the chemical industry. DA reactions of isoprene (1) and acrylic acid (2) (Scheme 1) have been investigated in both organic solvents and in pyridinium based ILs. The ionic liquid 1-ethyl-pyridinium trifluoroacetate [EtPy]⁺ [CF₃COO]⁻ is found to be an excellent reaction solvent with significantly increased rate for this reaction compared to conventional organic solvents.

In order to explain this experimental finding, theoretical investigation of the mechanism and the regioselectivity meta/para of this DA reaction have been carried out. The calculations have been performed in gas phase, in CH₂Cl₂ organic solvent and in 1-ethyl-pyridinium trifluoroacetate protic

IL. The reaction mechanism corresponding to the formation of the para regioisomers as major cycloadducts is elucidated by the analysis of the relevant stationary points of the potential energy surface and intrinsic reaction coordinate calculations. The calculation of activation and reaction energies indicates that the para cycloadducts are favored both kinetically and thermodynamically. The calculations, performed using explicit solvent model, show a considerable decrease of the activation barrier in the IL in comparison with gas phase and CH_2Cl_2 . The obtained results put in evidence the importance of hydrogen bonding formed between the IL and the dienophile fragment in the acceleration of this DA reaction. The calculations are carried out with the Gaussian 09 suite of programs using the B3PW91 exchange-correlation functionals together with the 6-31G(d,p) basis set and the obtained results are in good agreement with experimental outcomes.



Keywords: *Ionic liquid, Diels Alder reaction, mechanism, regioselectivity, solvent models, DFT study.*

PO 37

First principal investigation of Nowotney Chimney Ladder Silicide Ru_2Si_3 & Os_2Si_3

A. Cherifi, O. Benhelal, A. Chahed, H. Rozale, S. Laksari

Condensed Matter and Sustainable Development Laboratory, Physics Department

Djillali Liabès University of Sidi Bel-Abbès, Algeria.

hana55555@live.fr.

Abstract:

We present first principle calculations by the means of DFT (Density functional theory), using the Full-Potential Linearized Augmented Plane Waves (FP-LAPW) method inserted in the Wien2K code, of two Chimney-Ladder silicides Ru_2Si_3 and Os_2Si_3 . We will then emphasize the structural and electronic properties of these two materials through tables and figures to better understand interactions between atoms and particles that take place inside these two materials. Two approximations are used LDA (Local Density Approximation) & GGA (Generalized Gradient Approximation) to determine the exchange & correlation potential. We also applied mBJ (modified Becke-Johnson) potential to improve our results. It turned out that these two compounds are direct gap semiconductors. In general our results concerning lattice constants, and energy gap values, are in good agreement with experimental and theoretical results in literature. Alongside the electronic properties, we also calculated some optical parameters such as dielectric functions, Reflection coefficient, E-Loss and optical conductivity. In addition Ru_2Si_3 & Os_2Si_3 are considered as thermoelectric materials, as a result they may be very useful in new optoelectronic and thermoelectric applications.

Keywords:

PO 38

Molecular modeling evaluation of novel piperazine derivatives of flavones as potent anti-inflammatory agent

Ismail Daoud*, Amina Ghomri** and Abdelkrim Atmani***

* *Laboratoire des Substances Naturelles et Bioactives (LASNABIO). Département de Chimie, Faculté des Sciences Université Abou Bekr Belkaid de Tlemcen, Algérie*

daoud.ismail@yahoo.fr

** *École Préparatoire Sciences et Techniques Tlemcen, BP 165 RP Bel horizon ,13000 Tlemcen, Algerie*
am_ghomri@mail.univ-tlemcen.dz

*** *Département de Chimie, Faculté des Sciences, Université A. Belkaid, B. P. 119, Tlemcen, 13000, Algérie*

ab_atmanii@yahoo.fr

Abstract:

In this work a series of novel 6-methoxy-2-(piperazin-1-yl)-4H-chromen-4-one and 5,7-dimethoxy-2-(piperazin-1-ylmethyl)-4H-chromen-4-one derivatives of biological interest were studied. On one side B3LYP/6-31g(d) DFT level of theory calculations were used to obtain their molecular structures, the chemical reactivity parameters (electronegativity, hardness, electrophilicity and Fukui functions) that arise from Conceptual DFT. On other hand Molecular Docking is used to study the biological activity of these series of molecules. The calculated values were compared with the available experimental data for these molecules and discussed in terms of their usefulness in describing anti-inflammatory activities.

Keywords: Conceptual DFT, Molecular Docking, Pipérazine, Inhibitors, Anti-Inflammatory.

PO 39

Theoretical Study on Some Unnatural Amino Acids Used as Probing Molecules in Nonlinear Optics

S. N. Derrar^{*}, M. Sekkal-Rahal^{*} and P. Derreumaux^{**}

^{*} *Laboratoire de Microscopie, Microanalyse de la matière et Spectroscopie Moléculaire, Djilali Liabès
University, B.P. 89, Sidi Bel Abbès 22000, Algeria*

derrarsiham@yahoo.fr

majsekkal@msn.com

^{**} *Laboratoire de Biochimie Théorique, 13 Rue Pierre et Marie Curie, 75005 Paris, France*

philippe.derreumaux@ibpc.fr

Abstract:

Biological imaging is of a huge interest in the field of medicine. It allows analysing tissues and cellular functions. The well-known nonlinear optical (NLO) technique is widely used to perform biological imaging, mainly by means of second harmonic generation.

In the present work, the first hyperpolarizability (β) values of a series of unnatural amino acids are reported. Subsequently, the dipeptides formed by the combination of these unnatural amino acids and both tryptophan and lysine natural amino acids are investigated, respectively. The aim is to analyze the effect of such a combination in order to detect the suitable amino acids to be used as probing molecules in NLO.

Geometry optimizations are achieved with B3LYP functional, whereas MP2 method combined to 6-31+G(d) basis set is employed to calculate β . Gaussian03 program package is used.

Key words: Biological imaging, dipeptide, nonlinear optics, probing molecule.

PO 40

Synthesis Structures, cathecolase activité and Theoretical study of Schiff bases derivatives from DHA

A.Djedouani, N. Makouf and H. Boulemche

Laboratoire de Physicochimie Analytique et Cristallochimie des Matériaux Organométalliques et Biomoléculaires, Constantine 1.

djedouani_amel@yahoo.fr

naouel.makouf@yahoo.fr

ha_boulemche@yahoo.fr

Abstract:

Schiff bases are widely used as ligands to coordinate various metal ions because of the good solubility of their complexes. These compounds contain several donor atoms and have potential application in water treatment, due to their ability to readily form transition metals complexes. These complexes species are also involved in enzymatic reaction and present in proteins from conjunctive tissu. They can also be used as selective membranes or as corrosion prevent compounds. Our work is dedicated for the synthesis, characterisation and electrochemical study survey of new schiff bases, derivative from dehydroacetic acid (DHA : : 3-Acetyl-6-methyl-2H-Pyran-2,4(3H)-dione). and anilin and 4-chloro aniline respectively : (L1)=(E)-6-methyl-2-oxo-3-[1-(p-chloriminio)ethyl]-2H-pyran-4-olate, and L2=(E)-6-methyl-2-oxo-3-[1-(iminio)ethyl]-2H-pyran-4-olate. These two products were characterised by usual spectroscopic methods so as IR, NMR, and RX. The two molecules have a zwitterionic form with cationic iminium and anionic enolate groups.

An electrochemical study, by cyclic voltammetry for the two compound, has been achieved in aprotic medium, DMF-TBAHFB 0.1M, on a platin electrode of 2 mm of diameter. A cyclic sweep in the -1.8 to +1.8 V range shows for (L1) an anodic peak at 1.43V and two cathodic peaks at -0.717 V and -0.149 V. in the case of the (L2) and anodic peak at 0.13V and a cathodic peak appears at -0.147 V.

A theoretical study of such ligands were also investigated with a good correlation aspect using Density Functional Theory (DFT).

Key words: Cyclic voltammetry, Theoretical study, Schiff base, Zwitterionic.

PO 41

Study of the transfer of charge in the molecules combined by the methods of quantum chemistry

F. Djilali-Kobibi and M. Sekkal-Rahal

L2MSM laboratory - Faculty of Exact Sciences Djilali Liabes University. 22000. Sidi Bel-Abbes. Algeria

djilani.kobibifatma@yahoo.fr

majsekkal@msn.com

Abstract:

Cluster model structural and energetic calculations have been performed by means of *ab initio* and DFT methods. The aim is to examine electronic properties and more precisely the charges transfer for different structures. All structures corresponding to the cases were Intermolecular interaction energies of parallel (N-p-hydroxybenzylidène) Fig.1. were calculated with MP2, HF, B3LYP. The distance between the H atom of the monomere 1 and the monomere 2 increases from 4 Å to 6 Å.

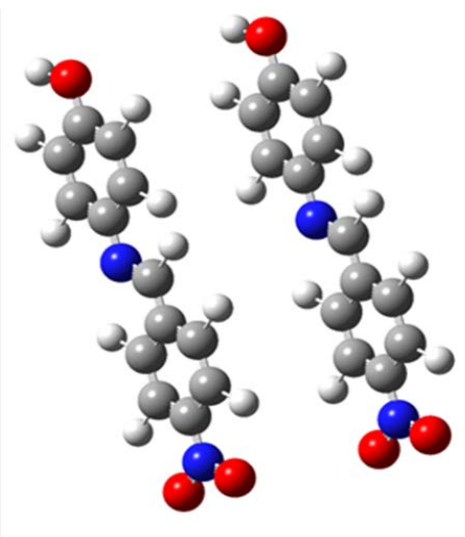


Fig.1 Different translations of cluster, using the DFT and MP2 methods

Key words: DFT, MP2, HF.

PO 42**Substitution effect of DPA on intramolecular charge transfer in presence of solvent. CIS-IEFPCM investigation**

Abdelkader M. El Horri and Majda Sekkal-Rahal

*L2MSM laboratory - Faculty of Exact Sciences Djilali Liabes University. 22000. Sidi Bel-Abbes. Algeria***a.melhorri@yahoo.fr**
majsekkal@msn.com**Abstract:**

Physicochemical properties of π -conjugated organic systems have attracted the attention of researchers in recent years. This is due to the fact that these molecules have effective properties in the fields of photonics and optoelectronics. Such systems include an organic conjugated backbone (chromophore) bound by a donor (D) and an acceptor (A) group. We focused our work on diphenyl acetylene molecule substituted by various donor groups such as NH₂, O-Meth, Eth-O, N-(Meth) 2 and acceptor groups like NO₂, CN, COOC. This groups are in para positions. The geometries and the electronic transitions of derivatives mentioned above have been investigated by the CIS / method 6-311 + g (d, p). The relationship between the structure, the electron transitions, the effect of the substitution of the molecule of interest and the effect of solvent were discussed. The effect of solvent on electronic transitions and charge transfer DPA derivatives have particularly been of interest, hence the calculations were done by the method IEFPCM-CIS / 6-311 + G (d, p).

Key words: intramolecular charge transfer (ICT), DPA chromophore, Push-pull molecules, Quantum Mechanics, solvent effects.

PO 43

Technical and Economic Aspects of hybrid photovoltaic-wind system for feeding a domestic house

B.Fellah, B.Benyoucef and A.Benseddik

*Research Unit Materials and Renewable Energy, Department of Physics
University of Abou Bekr Belkaid-Tlemcen, BP: 119 Tlemcen 13000, Algeria.*

bou19boum@gmail.com

benyoucef_boumediene@yahoo.fr

a_benseddik2008@yahoo.fr

Abstract:

We present in this work, a method for design and optimization of the size of the PV-wind hybrid energy system, for two different climate-sites in Algeria: Tlemcen and Bouzaréah. This method is based on annual monthly values, solar radiation and wind speed at the two sites available, to be able to supply energy at a constant power demand, domestic home study that is: 2,547 KWh/j (winter season) and 3,027 KWh/j (summer season). The results show on one hand, Photovoltaic system that is most appropriate for both sites, in relation to wind energy system due to the high solar potential, and secondly, the site of Tlemcen has a cheaper cost of hybrid energy system than the site Bouzaréah.

Key words: Photovoltaic system, Wind system, Storage System, Sizing, Optimization.

PO 44

Interaction of iota- and kappa-carrabiose with monovalent cations studied by DFT

Amina Fezazi and Majda Sekkal

Laboratory of Microscopy, Matter Microanalysis and Molecular Spectroscopy (L2MSM) University of Sidi-bel-Abbes, Algeria
fmouni-84@hotmail.fr

Abstract:

Carrageenans are linear sulphated polysaccharides occurring as cell wall constituents of red algae and are used as texturing agents in the food industry. The polymer backbone is composed of alternating α (1 \rightarrow 3) and β (1 \rightarrow 4) units. The objective of our study is mainly to explore the conformational space and identify conformations corresponding to the lowest energies taking into account the geometrical parameters such as the dihedral angles related to the glycosidic bond and the different orientations of the hydroxymethyl and hydroxyl groups present in their structures in the presence of potassium cation. To achieve this goal, the DFT methods were used in the study of the structures of \square and \square carrabiose especially in the gas phase and in solvent using the PCM implicit model. The main results showed a significant effect of the presence of the ion on the relative energy. However, the conformation of the hydroxymethyl group does not seem to affect their stability.

Key words: κ -carrabiose, ι -carrabiose, méthode DFT, B3LYP, minima, solvant implicite.



PO 45

New theoretical investigation on the electronic structure and magnetic interaction for both perovskites cubic SrFeO_3 and CaFeO_3 oxides

Filali Sihem, Hamdad Noura, Rozale Habib and Benhelal Omar

*Condensed Matter and Sustainable Development Laboratory, University of Sidi Bel-Abbes, Sidi Bel-Abbes
22000, Algeria*

omar_benhelal@yahoo.fr

Abstract:

The perovskites oxides with ABO_3 formula have attracted a growing importance for most scientific researchers in different technological applications, because they received a greatest interesting theoretical and experimental studies. Recently, they have shown a remarkable development in the magneto electronics and spintronics devices, also they are investigated in high capacity memories (HCM), dynamic random access memories, catalytic electrodes fuel cells, optoelectronics, sensors, laser frequency doubling, waves guides, non-volatile memories, laser host crystals, high kcapacitors, solid fuel cell, gas separation membranes, chemical reactors. Very recently, the spin effect and the magnetic interaction in the solid have played an important role to show specifics properties for sciences material, especially for the magnetic oxides with AFeO_3 or AMnO_3 systems (Fe–O–Fe, Mn–O–Mn bonds), whereas the magnetic moment coexist and gives differences between structures and solids. For more comprehension, we investigate both SrFeO_3 and CaFeO_3 oxides to show their structural, electronic and magnetic properties also we give a special attention to the spin effect using a comparison between two approaches GGA and GGA + U based respectively on the DFT and DFT + U theories. The U-Hubbard Hamiltonian added in the DFT + U basis has ameliorated the obtained results. The magnetic moment for different magnetic configurations (ferromagnetic FM, A-type anti-ferromagnetic A-AFM, and G-type anti-ferromagnetic G-AFM) for the cubic structure is discussed. The equilibrium lattices (a , c in Å), bulk modulus (B , in GPa), and its pressure derivatives (B_0) are computed, the present results agree very well with the theoretical and experimental data. The GGA + U is more efficient than the GGA. Both oxides SrFeO_3 and CaFeO_3 exhibit the G-AFM behavior.

Key words: Magnetic intermetallic, Magnetic properties, Ab initio calculation, Electronic structure.



PO 46

On the importance of the BSSE-CP correction during optimization of κ -carrabiose-water complexes

R. Fodil and M. Sekkal-Rahal

Laboratoire L2MSM, Faculté des Sciences. Université Djillali Liabes de Sidi Bel Abbas, B.P. 89. 22000 Sidi

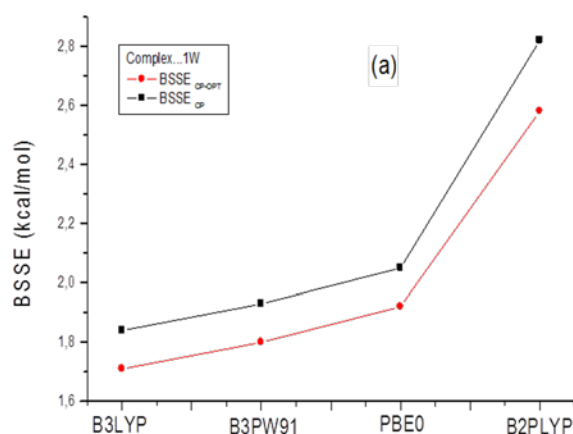
Bel Abbas. Algeria

rachafod@yahoo.fr

majsekkal@msn.com

Abstract:

Three κ -carrabiose-water complexes were geometry optimized at the B3LYP/6-31+G*, B3PW91/6-31+G*, PBEPBE/6-31+G* and B2PLYP/6-31+G* levels of theory. The BSSE (Basis Set Superposition Error) Counterpoise Correction (CP) was included during and after the optimization. The results derived from this study reveal that the inclusion of the BSSE-CP correction during the optimization is useless for all complexes.



Plots of the BSSE_{CP-CP} and BSSE_{CP} versus the different functional, BSSE_{CP-CP} and BSSE_{CP} are the BSSE values computed with and without including BSSE-CP correction during optimization, respectively.

Key words: Basis Set Superposition Error (BSSE), κ -carrabiose, disaccharide, CounterPoise (CP) correction, DFT methods.

PO 47

Half-metallicity in the half-Heusler RbSrX compounds (X= C, Si, Ge)

Gheriballah Slimane, Rozale Habib, Mesri Dalila and Benhelal Omar

*Condensed Matter and Sustainable Development Laboratory, University of Sidi Bel-Abbes, Sidi Bel-Abbes
22000, Algeria*

omar_benhelal@yahoo.fr

Abstract:

Half-metallic ferromagnets represent a new class of materials which absorbed a lot of attention due to three unique properties, Firstly, half-metals, have only one spin channel for conduction: the spin-polarized band structure exhibits metallic behavior for one spin channel, while the other spin band structure exhibits a gap at the Fermi level. Due to the gap for one spin direction, the density of states at the Fermi level has, theoretically, 100% spin polarization. Secondly, magnetic shape memory effect, where the magnetic shape memory alloys undergo structural transformations by changing the magnetic field. Thirdly, the inverse magnetocaloric effect, where some magnetic materials possess a reversible change in temperature caused by exposing the material to a changing magnetic field. Until now a lot of half-metallic ferromagnets are known. Full-Heusler and half-Heusler alloys are the most prominent among the half-metallic compounds. The full-Heusler alloys with the generic formula X_2YZ , where the X and Y sites are transition metals, and Z are sp elements, were proposed first by Heusler in 1903, and have attracted much attention due to their diverse physical properties and potential applications. Since the half-metallicity is discovered in some of these compounds, increasing investigations are being piled up all the times. In this paper, we use the first-principles calculations to investigate the structural, electronic and magnetic properties of the RbSrC, RbSrSi and RbSrGe compounds in the half-Heusler structure. It is found that ferromagnetic phase have lower energies than the antiferromagnetic and non-magnetic one for three compounds. Electronic structure and magnetic properties based on density functional theory (DFT) within the generalized gradient approximation (GGA) for RbSrX (X=C, Si, Ge) half-Heusler compounds have been performed using the full-potential linearized augmented plane wave (FP-LAPW+lo) method. The electronic band structures and density of states of three compounds show that the spin-down electrons have metallic, and the

spin-up bands have a gap of 1.73, 1.61, and 1.23eV for RbSrC, RbSrSi, and RbSrGe respectively, resulting in stable half-metallic ferromagnetic behavior with magnetic moments of $1\mu_B$.

Key words: Half-Heusler compound, Alkali metal, Ferromagnetism, Density functional theory.

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PO 48

The Dipole Moment, Polarizabilities, and First Hyperpolarizabilities of D/A Metal Porphyrins. A Comparative and Computational Study.

Mahfoud Hadj-benali*, Amar Saal** and Ourida Ouamerali*

**Laboratoire de Chimie Théorique Computationnelle et Photonique (LCTCP)*

Faculté de chimie, USTHB BP 32000 El Aalia, ALGER

m_hadjbenali@yahoo.fr

ouameralio@hotmail.fr

***Department of Chemistry, UMMTO University, Tizi-ouzou 15000, Algeria*

Abstract:

The development of chromophores for nonlinear optics (NLO) has been driven by a multitude of important technological applications that can be realized if suitable materials are available.

We present a quantum-chemical analysis of the central metal ions' effect on electronic structure, dipole moment (μ), electronic and vibrational polarizabilities (α) and first hyperpolarizabilities (β) of a set of donor-acceptor (D/A) metal porphyrins. The results, evaluated with the B3LYP/6-31G (d, p) model, have been compared to those of the typical chromophore, *para*-nitroaniline. This study contributes to highlight the effect that the central metal ion has on the two contributions to the first hyperpolarizability.

Key words: first hyperpolarizability, donor-acceptor metal porphyrins.

PO 49

Theoretical study of structural and nonlinear optical properties of cyclic phosphazenes

Djebar Hadji and Ali Rahmouni

Laboratoire de Modélisation et de Méthodes de Calculs- Centre Universitaire de Saida, B.P. 138, Cité En-Nasr-20002- Saida – Algérie.

Abstract:

Phosphazenes are a compounds having structure with a alternating of phosphorus and nitrogen atoms. Allcock et al [1] have synthesized the first stable polyphosphazene in 1965. Since, examples of these compounds have been reported in the litterature. They can be used as fire resistant. They have other applications based on their nonlinear optical properties (NLO) [2-4]. The NLO properties are consequences of the electronic and internal nuclear motions. All of them govern nonlinear optical NLO behavior. In general the electronic contribution is more important, but some materials present a more important vibrational contribution.

In this work, we are interested in structural and non-linear optical properties of series of cyclic phosphazenes. Our studies are based on HF and density functional theory (DFT) calculations with the functionals CAM-B3LYP and B3PW91, and using different base sets.

The first vibrational hyperpolarizability of these molecules was calculated at HF, DFT/CAM-B3LYP and DFT/ B3PW91 level of theory using 6-31G* and 6-31++ G* basis sets. These cyclic phosphazenes adopts a planar structure. The obtained results reveal that the cyclic phosphazenes derivatives have large vibrational hyperpolarizability.

Keywords: phosphazenes, polarizability, hyperpolarizability, NLO, HF, DFT.

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PO 50

Gas effect on the emission of backscattered electrons in an HPSEM

Hafsi Zoulikha, Mansour Omar and Kadoun Abd-Ed-daïm

Laboratory of Microscopy, Matter Microanalysis and Molecular Spectroscopy (L2MSM)

University of Sidi-bel-Abbes

aya.magister@yahoo.fr

momaro2002@yahoo.fr

Abstract:

In the scanning electron microscope system with the presence of gases (HPSEM), the incident electron beam is scattered by the gas molecules, forming the so-called 'skirting', when it travels through the gas to reach the specimen. While a large fraction, 50 % or more, of the beam current can be transferred from the focused beam to the skirt due to gas scattering, the electron current density at any point in the skirt is much lower than that in the focused beam. When a conventional electron image is formed by scanning such a beam/skirt combination over an array of pixels, it is the high current density of the focused beam that produces sharp responses across fine details of the specimen topography and creates a high resolution image. The skirt, which can even contain the majority of the beam electrons, is so spread out and locally diffuse that during a scan, particularly at high magnification, the skirt barely moves relative to the fine features that form the interesting image details. The gas-scattered skirt component is so widely spread that the electron imaging signals it produces are completely decoupled from the local imaging environment experienced by the focused beam. In the case of imaging with backscattered (BSE) or secondary electrons (SE) the skirt electrons produce a non specific signal that acts to increase the noise and degrade the signal-to noise ratio. Also a chemical characterization problem could arise when X-rays are generated by the scattered electrons from a nearby material that is different in composition from the interested material under the primary beam.

This work is dealing primarily with Monte Carlo simulation. It is interested in the electron-material interaction in the high pressure scanning electron microscopy (HPSEM) and in the effect of the gas on the backscattered electrons production from dielectric materials, in particular SiO₂ oxide.

Two gases were chosen; helium, for its well-known ability to reduce the skirt, and water vapor, for its high ionization efficiency. The systematic study of the backscattered electrons distribution proved that the presence of gas changes this distribution and effect on the interaction volume ,In particular, the radius of the exit zone of the backscattered electrons is significantly increased.

Key words: High pressure SEM, Monte Carlo simulation, electron-material interaction

PO 51

Study by molecular modeling opportunities adsorption of Desethyl-s-Atrazine and Desisopropyl Atrazine on montmorillonite

Hallouch Mustapha, Benahmed Abelatif and Zizi Zahia

Laboratory of Materials and Catalysis, Chemistry Department, Faculty of Sciences, Hai larbi Ben M'hidi BP 89 University of Sidi- Bel – Abbas; SIDI BEL ABBES, 22000, Algeria.

hallouchmustapha@yahoo.fr

z_zahia@yahoo.com

Abdellatif.Benahmed @ yahoo.fr

Abstract:

Technological development has led to a multitude of chemicals such as pesticides used in the fields of agriculture to improve crop yield. However, these products are not biodegradable and can all be found at the end of the cycle in surface water, groundwater and water reserves for consumption. The triazine group is one of the constituents that pose a great danger to humans. In this work, we conducted one hand, molecular mechanics calculations to optimize the geometry and minimize energy of desethyl -s-Atrazine ($C_6H_9ClN_5$) and Desisopropyl-s-Atrazine ($C_5H_8ClN_5$). On the other hand, we have calculated the size of the molecular dynamics pollutants studied to investigate the possibility of their adsorption on five types of montmorillonite (Mt (natural), Mt (Na), Mt (Ca), Mt (K) and Mt (Mg)). The results of our calculations showed that the adsorption of these pollutants on Mt (Na) and Mt (K) is impossible, whereas in other types of montmorillonite is possible.

Keywords: Clays, pesticides, montmorillonite, adsorption, the triazine group, the molecular dynamics, the molecular mechanics.



PO 52

Structure and physical-chemistry property relationship for indole derivatives

Harkati Dalal, Belaidi Salah and Rouahna yasmine

*Faculty of Sciences, LMCE Laboratory, Department of Chemistry, Group of Computational and
Pharmaceutical Chemistry, University of Biskra, 07000, Biskra, Algeria*

harkatidalal@yahoo.fr

rahouyasmine@yahoo.fr

salah_belaidi@hotmail.com

Abstract:

The indole structure represents a highly relevant hetero-cyclic system, since numerous products natural and synthetic containing indole. Indole derivatives constitute an important class of therapeutic agents in medicinal chemistry including anticancer, antioxidant, and also antirheumatoid and anti-HIV. Moreover, it has been demonstrated that introduction of heterocyclic moieties such as isothiazoles at position 3 of the indole nucleus can enhance these biological activities.

Quantum chemistry methods play an important role in obtaining molecular geometries and predicting various properties. To obtain highly accurate geometries and physical properties for molecules that are built from electronegative elements, expensive *ab initio*/HF electron correlation methods are required. Density functional theory methods offer an alternative use of inexpensive computational methods which could handle relatively large molecules.

As one of the most powerful techniques for predicting the bioactivity of various molecules, QSAR starts only with the molecular structure information of the previously reported active molecules. The parameters physic-chemical approach offers important insight into the relationships between the molecular structure and biological activity of the investigated compounds.

Here we investigate the quantitative structure activity relationships of a series of Indole derivatives reported in literature as inhibitors of hepatitis C compounds. The calculated results have been reported in the present work. Results and discussion.

Key words: Activity, indole, molecular, QSAR, quantum chemistry.

PO 53

On natural convection in an open geometry

Yamina Harnane

*Université Larbi-ben-M'hidi, Faculté des Sciences et Sciences appliquées, Département de Génie
Mécanique, Oum-El-Bouaghi, Algérie*

harnane_y@yahoo.fr

Abstract:

The CFD code, Fire Dynamic Simulator (FDS) was used to model natural convection in a 2D vertical channel with a heated square bar. The unsteady, turbulent, and incompressible flow is assumed to investigate the natural convection heat transfer over the square bar mounted near the left wall of the channel. The calculation of the thermal turbulent flow field with the LES requires obtaining the solution of the governing equations. The fluid is assumed to enter into the channel at ambient temperature T_0 . The channel walls are maintained at uniform temperature T_w , while the square bar surface temperature is at T_b . One type of boundary conditions is used in the calculations (Dirichlet): free boundary conditions at the inlet and outlet surfaces notified by “OPEN” in the code FDS. Numerical calculations are made for the modified Rayleigh number Ra_m changed between 4×10^7 and 10^8 . The results study included mean velocity profiles presented in dimensionless form as well as, flow structure and Nusselt number profiles.

Key words: Computational Fluid Dynamics, Natural Convection, Turbulent Flow

PO 54

Higher Order Boundary Valued Problem for Impulsive Differential Inclusions

Johnny Henderson^{*}, Abdelghani Ouahab^{**} and Samia Youcefi^{**}

^{*} *Department of Mathematics, Baylor University Waco, Texas 76798-7328 USA*

Henderson@baylor.edu

^{**} *Laboratory of Mathematics, Sidi Bel Abbès Université PoBox 89, 22000 Sidi Bel Abbès, Algerie*

agh_ouahab@yahoo.fr

youcefi.samia@yahoo.com

Abstract:

Many properties of solutions for differential equations, such as stability or oscillation, require global properties of solutions. This is the main motivation to search for sufficient conditions that ensure global existence of solutions for impulsive differential equations and inclusions. In this direction, this work deals with the existence results of solutions for the higher order differential inclusions with impulse effects and boundary conditions on an unbounded domain.

Our goal in this work is to give some existence results when the right-hand side multi-valued nonlinearity can be either convex or nonconvex. We will treat two cases, in the first we give an existence result based on nonlinear alternative of Leray-Schauder type for condensing upper semicontinuous multi maps (the convex case). In the nonconvex case, we present the second existence result for the considered problem when the multi-valued nonlinearity is not necessarily convex. In the proof, we will make use of the nonlinear alternative of Leray-Schauder type combined with a selection theorem due to Bressan and Colombo for lower semicontinuous multi-valued maps with decomposable values. Also, another result is presented as an application of the fixed point theorem for contractive multi-valued operators given by Covitz and Nadler.

Key words: decomposable set, fixed point, multi-valued maps, impulsive differential inclusions.

PO 55

FDTD Modeling of Silicon-based Photonic Crystals

A. Dekhira, K. Zellagui and O. Ouamerali

*Faculté de Chimie, Laboratoire de Chimie Théorique Computationnelle et Photonique, USTHB, El Alia
16111 Bab Ezzouar, Alger, Algérie*

azedbox@gmail.com

kheirouzell@yahoo.fr

ouameralio@hotmail.fr

Abstract:

Photonic crystals are periodic optical nanostructures that are designed to affect the motion of photons in a similar way that periodicity of a semiconductor crystal affects the motion of electrons. As Silicon is the dominant material in the microelectronics, it would be highly advantageous to also use silicon as a key material for silicon-based photonics. The main objective of this work is the development of an efficient finite-difference time-domain (FDTD) scheme, optimized for silicon-based photonics. This approach requires the implementation of linear dispersion and nonlinear Kerr and Raman effects in FDTD by auxiliary differential equation (ADE). Auxiliary differential equation methods extend the FDTD technique to incorporate polarization by time-stepping auxiliary differential equations with Maxwell's curl equations and extend FDTD time steps beyond the conventional Courant-Friedrichs-Lewy stability limit. The corresponding code is developed using the programming language C++ through the multiplatform framework QT as well as a selection of scientific libraries and templates. A modular approach is adopted to enable code reuse and ease of upgrade in future. The code was validated by performing several test-cases for 1D and 2D Silicon-based media. Our results show higher computational efficiency, as compared to the results obtained by a conventional FDTD method.

Key words: FDTD method, Photonic crystals, QT framework, Silicon photonics.

PO 56

Lipophilic efficiency Analysis and Comparison of Drug Efficacy of Triazolothiadiazole Derivatives by QSAR Analysis

Kerassa Aicha, Belaidi Salah and Harkati dalal

Faculty of Sciences, LMCE Laboratory, Department of Chemistry, Group of Computational and Pharmaceutical Chemistry, University of Biskra, 07000, Biskra, Algeria.

aichachimie1@gmail.com

prof.belaidi@gmail.com

harkatidalal@yahoo.fr

Abstract:

Quantitative structure activity relationship (QSAR) methods have been applied in several scientific studies including chemistry, biology, and toxicology and drug discovery to predict and classify biological activities of virtual or newly-synthesized compounds.

To rationalize the drug discovery/development process and to guide the optimization from lead compound to successful drug candidate, rules for predicting drug-like physio-chemical properties have been introduced. The Lipinski's 'Rule of Five' as well as other parameters like lipophilic efficiency (LipE) have been shown to be useful tools to aid in choosing oral drug candidates.

An important objective for this research was to evaluate the physicochemical domain of the twenty triazolothiadiazole derivatives reported in literature has a biological activity, some of physicochemical properties were calculated using HyperChem 8.03 software and others were calculated using Molinspiration online database .

We find that the triazolothiadiazole derivatives exhibited a great %ABS, which indicating that these compounds should have good cellular plasmatic membrane permeability. And, all these derivatives were flexible, especially, compounds 1-6 which have 5 rotatable bonds.

All compounds meet the Lipinski rules of the five, suggesting that these compounds theoretically would not have problems with oral bioavailability.

The compound 2 had the highest LipE value of the data set and was deemed to be the most optimal compound.

Key words: LipE, Lipinski's 'Rule, QSAR, Triazolothiadiazole derivatives.

PO 57

Ab Initio Study of Structural, Elastic, electronic and thermal Properties of Full Heusler Compounds Fe₂VX (X=Al, Ga)

M. Khalfa^{*/**}, H. Khachai^{***} and K. Bougherara^{*}

^{*}: Physics Department, Djillali Liabes University of Sidi Bel-Abbes, Algeria

^{**}: Commissariat à l'Energie Atomique, Centre de Recherche Nucléaire de Draria (CRND). B.P: 43, Draria, Alger, Algeria

m_khalfa10@yahoo.fr

^{***}: Applied Materials Laboratory (AML), Physics Department, Djillali Liabes University of Sidi Bel-Abbes, Algeria

Abstract:

Recently lattice properties and electronic structure calculations have become very important in the fields of physics and chemistry for almost 40 years ago. Ternary Fe₂VZ (Z=Al, Ga) intermetallic represents part of heusler family [1] type X₂YZ compound where X and Y are transition metals, and Z is a main group element which crystallize in in cubic L21 structure, The most important characteristics of these ferromagnetic compounds are their very high Curie temperature and their half metallicity. The Fe₂VAl and Fe₂VGa intermetallics have recently attracted great attention due to their unusual magnetic, transport, electrical and thermal properties [2-3-4-5-6], A theoretical study of structural, elastic, electronic and thermodynamic properties of Fe₂VX, with X = Al and Ga, were studied by means of the full-relativistic version of the full-potential augmented plane wave plus local orbitals. We employed both within the generalized-gradient approximation (GGA) and local-density approximation (LDA) for exchange and correlation.

We note that GGA appear more accurate than LDA in calculating the structural properties and we will use it in all calculations in this study. The ground state properties, lattice constants, bulk modulus and elastic constants agree well with available experimental and theoretical data. Thermal effects on some macroscopic properties of Fe₂VX are predicted using the quasi-harmonic Debye

model in which the lattice vibrations are taken into account. We have obtained successfully the variations of the primitive cell volume, volume expansion coefficient, heat capacities and Debye temperature with pressure and temperature in the ranges of 0–40 GPa and 0–1500 K. For the first time, the numerical estimates of the thermal properties are performed for Fe₂VX with X = Al, Ga.

Keywords: Full Heusler, FP-LAPW, electronic properties, thermal properties

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- thods.



PO 58

FP-LMTO calculations of the structural, elastic, thermodynamic and electronic properties of the ideal-cubic perovskite BiGaO_3 .

A. Kourdassi , M. Benkabou , N. Benkhetrou and D. Rached

**Laboratoire des matériaux magnétiques Université Djillali Liabès 22000 Sidi Bel-Abbès, Algérie*
akourdassi@yahoo.fr

nordine_bt@yahoo.com

rachdj@yahoo.fr

Abstract:

Using the first principles full potential linear muffin-tin orbital method within the local density approximation, we have studied the structural, elastic, thermodynamic and electronic properties of the ideal-cubic perovskite BiGaO_3 . It is found that this compound has an indirect band gap. The valence band maximum (VBM) is located at Γ point, whereas the conduction band minimum (CBM) is located at X point. The pressure and volume dependences of the energy band gaps have been calculated. The elastic constants at equilibrium are also determined. We derived the bulk and shear modul, Young's modulus, and Poisson's ratio. The thermodynamic properties are predicted through the quasi-harmonic Debye model, in which the lattice vibrations are taken into account. The variation of the bulk modulus, heat capacities and Debye temperature with pressure and temperature are successfully obtained.

Key words: FP-LMTO, perovskite, thermodynamic properties.

PO 59

Theoretical studies on histamine tautomerism

Lafifi Ismahan and Khatmi Djameleddine

Laboratory of Computational Chemistry and Nanostructures. University of Guelma

lafifiismahane@gmail.com

khatmi.djameleddine@gmail.com

Abstract:

DFT calculations with different levels are applied to investigate the tautomer forms for the Histamine molecule induced by proton transfer in gas phase, in continuum solvent and in microhydrated environment with one, two and three explicit water molecule. The results obtained in this study show that the A form is the most stable tautomer. The relative stability in water is slightly modified when the system was described with PCM model (calculations carried out only with B3LYP). Finally, with monohydrate environment the calculations show that A tautomer is more stabilized due to its structure which allows further H-bond with water molecule.

Key words: histamine – tautomer – DFT –water complex – solvent and PCM model.

PO 60

Origin of magnetism in the sp-half metallic compounds

Abdelaziz Lakdja^{*}, Habib Rozale^{*}, Adlane Sayede^{**} and Abbès Chahed^{*}

^{}Condensed Matter and Sustainable Development Laboratory, Physics Department,
University of Sidi-Bel-Abbès, 22000 Sidi-Bel-Abbès, Algeria.*

alakdja@yahoo.fr

*^{**}UCCS, CNRS-UMR 8181, Université d'Artois, Faculté des Sciences Jean Perrin, Rue
Jean Souvraz, SP 18, 62307 Lens Cedex, France.*

Abstract:

Spin-polarization in systems without partially occupied d or f states attracts increasing research interest as potential materials in spintronic devices. A new class of materials based on alkali and alkaline earth metal-based materials show half-metallic character where the magnetic order is carried by the p states without any direct contribution of d electrons. Among this new class of materials, namely sp-half metallic ferromagnets, I-V, II-V, and II-IV compounds are extensively studied. We present a description of this new class of materials, and give the mechanism that underlies the coupling of the magnetic moments.

Key words: alkali and alkaline earth metals, ferromagnetism, density functional theory.

PO 61

Computational Analysis of Turbulent Mixing in Confined Swirling Flow

D. Lalmi and R. Hadeif

Université Larbi Ben M'Hidi, 04000 Oum El Bouaghi, Algérie

rhadeif@rocketmail.com

Abstract:

The mixing of fuel and air plays a significant role key in combustion systems with respect to pollutant formation and emissions and chemical reactions. For modern low-emission gas turbines, the level of mixing between fuel and oxidant prior to combustion is a crucial design parameter. For instance, lean well mixed low NO_x combustion is an essential feature of modern power generating gas turbines. Single digit NO_x emissions, in some case even below 3ppm, are now achievable without catalytic after-treatment but only with considerable optimization of the fuel/air mixing. Because of the great practical importance of mixing several methods such as numerical, analytical, and experimental analyses have been used to study and predict this phenomenon.

In the present work, the mixing of fuel and air in an isothermal high-intensity swirling flow in a model combustor has been examined computationally. The focus is on the Reynolds -averaged Navier–Stokes computations of the momentum and scalar transport employing turbulence models based on the differential second moment closure (SMC) strategy. Prediction results are validated against measurements.



PO 62

Conformational and Vibrational Study in the Gas Phase of some Amino Acids: Cysteine, Serine and Aspartic Acid

Abbassia Lazreg, Ilham Naoual Taleb-Mokhtari and Majda Sekkal-Rahal

Laboratoire de Microscopie, Microanalyse de la matière et Spectroscopie Moléculaire (L2MSM),

Département de Chimie, Faculté des Sciences, Université Djillali Liabes, B.P. 89, 22000,

Sidi Bel Abbès, Algeria

ablazreg@yahoo.fr

il_taleb@yahoo.fr

majsekkal@msn.com

Abstract:

Conformational study using DFT and ab initio methods was performed on three amino acids: cysteine, serine and aspartic acid. Each one of these acids is different from the two others by the radical group, which confers specific physicochemical properties. In fact, the orientations of the side chain may affect the stability and produce a large number of conformations.

The structures were optimized using the B3LYP/6-31G (d,p) method followed by an increase of the B3LYP/CCPVDZ, B3LYP/AUG-CCPVDZ bases. A total of 120 conformers were found for cysteine and 96 for both serine and aspartic acid. A multi-conformational search using the MP2/AUG-CCPVDZ method has helped to identify the lowest energy conformations including a conformation representing the global minimum. These lowest energy conformations were used as a basis to represent the forms in gas phase respectively used for the vibrational study of these amino acids. We undertook a calculation of frequencies in order to proceed with the attribution of certain characteristic vibration modes. The relative energies, rotational constants, dipolar moments, vibrational energies of point zero and of harmonic frequencies were calculated for the low energy conformers for each amino acid. In addition to the size, nature and orientation of the side chain characterizing each amino acid, the type of the intramolecular hydrogen bonds affects the frequencies of harmonic vibrations and causes a displacement of the vibration frequencies, accompanied also by an increase in intensity and a widening of the bands.

Keywords: amino acids, conformational study, conformer, vibrational spectra.

PO 63

A DFT study of the Regio- and Stereoselectivity of the Aza Intramolecular-Diels-Alder reaction yielding to the formation of the 5aH-chromeno [2,3-c]acridine

M. A. Mahi, W. Benchouk and S. M. Mekelleche

Laboratory of Applied Thermodynamics and Molecular Modelling, Department of Chemistry, Faculty of Science, University of Tlemcen, 13000, Algeria

awatifmahi@yahoo.com

sm_mekelleche@mail.univ-tlemcen.dz

Abstract:

The Intramolecular Diels-Alder (IMDA) reaction provides a powerful strategy for the construction of complex carbocyclic and heterocyclic systems in only one synthetic step. In this contribution, we present a theoretical study of the mechanism, regio- and stereoselectivity of the aza Intramolecular-Diels-Alder (IMDA) reaction of (E)-N-((2-(but-3-enyl)-2H-chromen-3-yl)methylene) benzenamine yielding the *trans*-fused chromeno [2,3-c] acridine. The calculations were performed at the B3LYP/6-31G(d,p) level of theory and the possible regio-(fused/bridged) and stereo-(*cis/trans*) isomeric channels to provide the different stereoisomers were thoroughly investigated. The free activation enthalpies, calculated in the presence of the BF₃ Lewis acid catalyst and acetonitrile solvent using the MPW1B95/6-31G(d,p) method, show that the formation of the *trans*-fused of chromeno acridine cycloadduct is favored both kinetically and thermodynamically as found experimentally. The fused regioselectivity has been also elucidated using the electrophilic and nucleophilic *Parr* functions. Intrinsic reaction coordinate (IRC) calculations and the topological analysis of the electron localization function (ELF) of some relevant points of the IRC curve show that the *trans*-fused favoured channel takes place via a one-step two-stage mechanism. Charge transfer calculations performed at the transition states in combination with the calculation of DFT-based reactivity indices of the diene/dienophile fragments of the reactant indicate a polar character of the studied reaction.

Key words: aza Intramolecular-Diels-Alder reaction; Regioselectivity; Stereoselectivity; Density functional theory.

PO 64

Existence results for prion diseases model

Imane Mammar, Abdelkader Lakmeche and Abdelghani Ouahab

Laboratory of Mathematics, Sidi-Bel-Abbes University, PoBox 89, 22000 Sidi-Bel-Abbes, Algeria.

i.mammar@yahoo.com;

lakmeche@yahoo.fr;

agh_ouahab@yahoo.fr

Abstract:

A model of prion evolution with impulse effects (MPI) is studied, by the mean of the evolution semigroup theory we prove existence and uniqueness of mild solutions for (MPI).

Key words: Impulsive differential equation, prion model, evolution semigroup, mild solution. 1

AMS (MOS) Subject Classifications: 34A37, 34A60, 34G20, 34G25

References:

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PO 65

DFT study of the degradation mechanism of the anticancer drug imexon in aqueous solution

N. Massout, D. Kheffache and O.Ouamerali

Doctoral School Physical Chemistry Theoretical Chemistry Computer Science Faculty of Chemistry

USTHB, BP 32 El Alia BabEzzouar, Algiers

nouara.massout@hotmail.fr

kheffache.djeff@gmail.com

ouameralio@hotmail.fr

Abstract:

Imexon (4-imino-1,3-diazabicyclo[3,1,0]-hexan-2-one) is a member of the class of 2-cyanoaziridine derivatives, which have been of interest as immunomodulators and anticancer agents since the late 1970s. Several studies investigating stability and degradation of imexon have shown that this drug decomposes in aqueous solution to produce the major degradation product (**DP**) represented in figure 1.

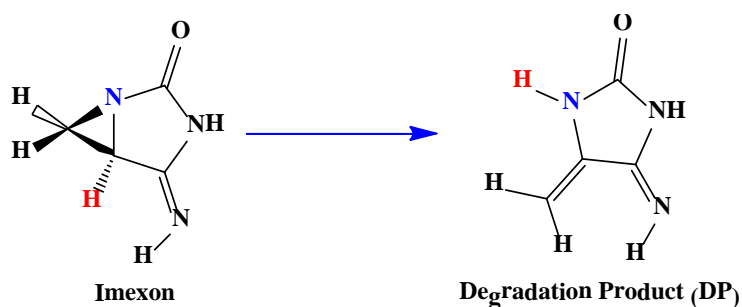


Figure 1: Degradation product of imexon.

Due to the risk that the degradation product (**DP**) may pose to the patients, the study of its mechanism of formation in aqueous solution is a critical step in understanding stability issues of imexon. In the present investigation, DFT calculations have been applied to elucidate the mechanism of degradation of imexon, in aqueous medium. We hope that our theoretical study will be helpful in understanding the stability of imexon essential for its pharmaceutical development.

Keywords: imexon, DFT, mechanism of degradation.



PO 66

Conformational analysis of l-carrabiose tg using semiempirical methods

N. Meçabih and M. Sekkal-Rahal

Faculté des sciences, Laboratoire L2MSM, Université Djillali Liabes de Sidi Bel Abbès, B.P.89, Sidi Bel Abbès, 22000, Algeria

nadia.mecabih@gmail.com

Abstract:

Energy surfaces were computed for the iota-carrabiose 4-O-sulphate- β -D-galactopyranosyl (1 \rightarrow 4), 2-O-sulphate 3,6 anhydro- α -D-galactopyranose.

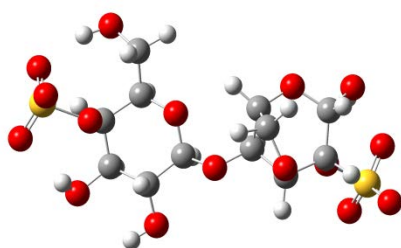


Figure 1: Structure of the ι -carrabiose 4-O-sulphate- β -D-galactopyranosyl (1 \rightarrow 4), 2-O-sulphate 3, 6 anhydro- α -D-galactopyranose

Figure 2: Relaxed iso-potential map using AM1 method of ι -carrabiose in the gas phase. (ΔE in kcal/mol)

Carrageenans are water-soluble sulfated galactans coming from marine red algae Rhodophyceae with alternating α -(1 \rightarrow 3) and β -(1 \rightarrow 4)-linked galactopyranosyl residues. Gelation by carrageenan has been considered to involve helical structures and aggregates of helices.

In this study, conformational maps were calculated for the iota-carrabiose 4-O-sulphate- β -D-galactopyranosyl (1 \rightarrow 4), 2-O-sulphate 3, 6 anhydro- α -D-galactopyranose (figure 1) in gas phase by using semi-empirical quantum mechanical methods (AM1). In this optimized structure both hydroxymethyl groups present a tg orientation. Relaxed conformational maps were also built for l-carrabiose (figure 2) by interpolating a set of data comprising 324 energy values, which was also generated by varying each dihedral angle in increments of 20°. In the gas phase we have obtained four minima for the l-carrabiose, corresponding to the lower energy conformers. We note that our lowest energy conformer A corresponds to the conformer of starting (-71°, 94°).

Key words: l-carrabiose; disaccharide; glycosidic linkage; energetic relaxed; semi-empirical methods.

PO 67

A DFT study of the Halogenation reaction in glutaconaldehyde benzoyl ester: Application of the static approaches of the chemical reactivity

A. Merouane, A. Mostefai and A. Rahmouni

*Laboratoire de Modélisation et de Méthodes de Calculs- Université de Saida, B.P. 138, Cité En- Nasr-
20002- Saida – Algeria.*

Abstract:

Glutaconaldehyde benzoyl ester is a bifunctional reagent where more than one site can be attacked, and, as such, a potential precursor for various heterocyclic compounds [1]. The present study is a theoretical investigation of the Halogenation reaction of glutaconaldehyde benzoyl ester with Fluorine, Chlorine and Bromine. This reaction was experimentally found to be regiospecific [2]. Because our main interest, in this work, is to predict which atomic site is the most susceptible to undergo an electrophilic attack, it will be sufficient to focus attention to the static approaches of the chemical reactivity. Indeed, the calculated reactivity indices derived from density functional theory which were used as an alternative to the traditional frontier orbital theory are applied to probe the local reactivity and site selectivity of the molecule under study. Fukui functions (FF), local softness and local philicity have been calculated from Mulliken population analysis (MPA) [3] and Hirshfeld population analysis (HPA) [4]. To improve the results accuracies, a large basis sets, such as 6-311+G(d) and 6-311+G(d,p) were used. The predictions thus made are in a good agreement with experimental results and theoretical calculations of the previously studied analogues.

Keywords: DFT, Fukui indices, Halogenation reaction, Transition state

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PO 68

Magnetic exchange coupling in $M^{II}_2 U(IV)$ Complexes ($M = Cu, Zn$). A relativistic DFT study.

Samir Meskaldji^{*/**}, Abdou Boucekkine^{***} and Lotfi Belkhiri^{*}

^{*}*Unité de Recherche Chimie de l'Environnement et Moléculaire Structurale (URCHEMS), Université de Constantine 1, 25017 Constantine, Algérie*

^{**}*IRAMIS, UMR 3299 CEA/CNRS SIS2M, CEA/Saclay, 91191 Gif-sur-Yvette, France*

^{***}*Laboratoire Sciences Chimiques de Rennes, UMR-CNRS 6226, Université de Rennes 1, Campus de Beaulieu, 35042 Rennes Cedex, France*

samirmeskaldji@yahoo.fr

lotfi.belkhiri@umc.edu.dz

abdou.boucekkine@univ-rennes1.fr

Abstract:

The development of molecular magnets materials, commonly called SMM (Single Molecular Magnet) is one of the newest areas of investigation of basic and applied research. The theoretical study of these magnetic systems, ferro or antiferromagnetic, is very useful. However, it requires the implementation of laborious calculation.

One of the critical points is the estimation of magnetic coupling constants J between metal centers. As part of the theory of density functional (DFT), the constant J is usually calculated from the energy difference between the state of high-spin (HS) and low spin state, obtained for the latter approach by broken symmetry (BS). We propose to study, using this methodology, various polynuclear complexes or mixed elements $f d / f$, potential candidates for SMM, including complex $M^{II}_2 U^{IV}$ ($M = Cu, Zn$).

Key words: Uranium(IV) complexes, Magnetic exchange coupling, ZORA/B3LYP, Broken symmetry.



PO 69

A CBS Study of 1-butene Reaction with Triplet Oxygen Atom O(³P)

B. Messaoudi^{*,**,***}, S. M. Mekelleche^{*} and N. Mora-Diez^{**}

^{*}: Laboratoire de Thermodynamique Appliquée et Modélisation Moléculaire, Département de Chimie,
Faculté des Sciences, Université de Tlemcen, BP 119, Tlemcen, 13000, Algérie

messaoudiboulanouar@yahoo.ca

sidi_mekelleche@yahoo.fr

^{**}: Department of Chemistry, Thompson Rivers University, Kamloops, BC, V2C 0C8, Canada

nmora@tru.ca

^{***}: Unité d'Analyse et Développement Technologique en Environnement, Centre de Recherche Scientifique et
Technique en Analyses Physico-Chimiques, BP 384, Bou-Ismaïl, 42004 Tipaza, Algérie

Abstract:

A theoretical study of the mechanism of the addition of the triplet oxygen atom O(³P) to 1-butene has been performed at the MP2, CBS-4M and CBS-QB3 levels of theory. The complex reactional mechanisms including both O-additions and H-abstractions are thoroughly investigated (**Figure 1-2**). The O(³P) can be added to either two carbon atoms of the double bond of the alkene and the less substituted end (**C1**) is only slightly preferred. Our calculations show that H + CH₃CH₂CHCHO (P1) and CH₂COCH₂CH₃ + H (P5) are major products. The calculated enthalpies at the CBS-QB3 level of theory are in very good agreement with experimental results and the O-addition is by far the most important reaction.

Key words: Atmospheric reactions, ground state oxygen, 1-butene, CBS methods

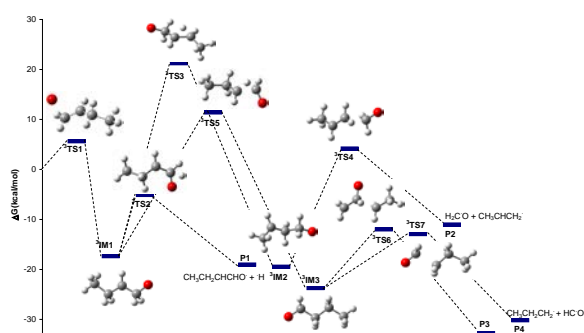


Figure 1: Addition on C1 carbon

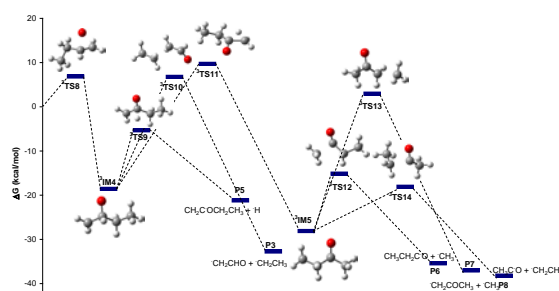


Figure 2: Addition on C2 carbon

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PO 70

Predictive study of physical properties of new multiferroic materials type ABO_3

Moulay Nouredine, Ameri Mohammed and Zenati Aziz

Laboratoire Physico-Chimie des Matériaux Avancés (LPCMA); Djillali Liabes University of Sidi-Bel-Abbes, 22000.Algeria

n_moulay@hotmail.com

az76ziz@yahoo.fr

lttnsameri@yahoo.fr

Abstract:

The full potential linear muffin-tin orbital method within the spin local density approximation is used to study the structural, electronic and magnetic properties of the three multiferroic compounds type ABO_3 . The large values are obtained for bulk modulus for these compounds, which demonstrates their hardness. A complex of strong hybridization is observed at Fermi level, due to the d state of the three compounds. The two degenerate levels e_g and t_{2g} clearly demonstrated the originality of this complex. We have also investigated the behaviour under pressure on the magnetic moments per atoms from 0 GPa to 55 GPa and the exchange magnetic energy between the ferromagnetic and ferrimagnetic states. For a more detailed knowledge, we calculated the thermodynamic properties. We have determined Heat capacity, Debye temperature, the bulk modulus and the Entropy through differentes temprature and pressions for the three multiferroic compounds. However, this is the first predictive calculations for all these properties.

Key words: electronic properties, structural properties, magnetic properties, thermodynamic properties.

PO 71

C-Mannosylation and O-Fucosylation

Hidayet Moulessehoul and Majda SEKKAL

Laboratoire L2MSM, Faculté des Sciences. Université Djillali Liabes de Sidi Bel Abbès, B.P. 89. 22000 Sidi

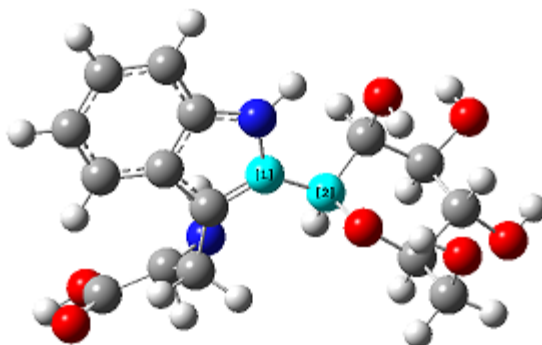
Bel Abbès. Algeria

h.mouless@hotmail.fr

majsekkal@msn.com

Abstract:

The purpose is to study the interaction of a specific peptide to a sugar with quantum mechanics methods for C-Mannosylation and O-Fucosylation. The C-mannosylation is a type of protein glycosylation involving carbon - carbon bond between mannose and a tryptophan residue of Trp-x-x-Trp sequence.



The O-Fucosylation is the addition of carbohydrate residues at the hydroxyl group of serine and threonine amino acids of peptide bonds. This preliminary study will help to identify the stability of a small fragment and could easily be transferred to larger systems in which the configuration of the transition state remains to be determined. For the optimization of the Tryptophan-mannose and Serine-fucose, we applied the B3LYP 6-31g(d) and 6-31g+(d), the energetic calculations lead us to draft their energies with various existing interactions. The frontier molecular orbital theory (FMO) and Fukui parameters have been used to identify the active sites of the two fragments. Then, we focused our study on a larger system, based on Trp-x-x-Trp sequence for C-mannosylation, and O-fucosylation was targeted β 1, 3 Glc-Fuc- α 1-O-Ser found in human urine.

Key words: Amino acid, Interactions, Peptides, Saccharide.

PO 72

Influence of the magnetization damping on Magnetic Susceptibility and Dynamics Hysteresis loops of biaxial nanoparticle

B.Ouari*, L. Méchernène* and Y.P.Kalmykov**

*University of Tlemcen, Physics department, BP 119 Chetouane, Tlemcen, Algeria.

**Univ. Perpignan Via Domitia, Laboratoire de Mathématiques et Physique, EA 4217, F-66860, Perpignan, France.

b.ouari@voila.fr

l_mechernene@yahoo.fr

Kalmykov@uni-perp.fr

Abstract:

The nonlinear susceptibility $\chi_1^1(\omega)$ and dynamic magnetic hysteresis (DMH) [1] of single domain ferromagnetic particles with biaxial anisotropy $\beta V = (\sigma + \Delta \cos^2 \varphi) \sin^2 \vartheta$ [2] induced by an external ac field of arbitrary strength and orientation are treated via Brown's model of coherent rotation of the magnetization [3] ($\sigma = \beta K$, K is the anisotropy constant, Δ is the biaxial parameter, $\beta = v / (kT)$, v is the volume of the particle, k is Boltzmann's constant, T is the absolute temperature, ϑ and φ are the polar and azimuthal angle, respectively). We demonstrated that the nonlinear ac stationary response and DMH strongly depend on the damping parameter, the ac field and the biaxiality parameter Δ .

Key words: Magnetic Nanoparticle, Brown Model, Fokker Planck Equation, Dynamic Magnetic Hysteresis (DMH)

PO 73

Molecular structure, Vibrational frequencies and frontier molecular orbital calculations on $C_{20}H_{15}S_3N_2O_2F$ compound using Hartree Fock and Density Functional Theory

R. Rahmani*, K. Toubal **, A. Chouaih* and F. Hamzaoui *

*Laboratory of Technology and Solid's Properties, Faculty of Sciences and Technology, BP227, Abdelhamid Ibn Badis University, Mostaganem 27000, Algeria

rahmani_ra63@yahoo.fr

ack_chouaih@yahoo.fr

fodil_hamzaoui@yahoo.fr

** Laboratoire de Synthèse Organique Appliquée (LSOA), Département de Chimie, Faculté de Sciences, University of Oran-Es-Sénia, 31000 Oran, Algeria

genekhaledo@yahoo.fr

Abstract:

In the present study, the structural properties of 3-(4-fluorophenyl)-5-(3-(2-methoxyphenyl)-4-methylthiazol-2(3H)-ylidene)-2-thioxothiazolidin-4-one have been studied using ab initio Hartree-Fock (HF) and density functional theory (DFT) at B3LYP exchange correlation with 6-31G(d,p) basis set. The Fourier-transform infrared (FT-IR) spectrum of the title compound has been recorded in the region 4000-400 cm^{-1} . The harmonic vibrational frequencies were calculated and the scaled values have been compared with experimental FT-IR spectrum. The complete assignments were performed on the basis of the total energy distribution (TED) of the vibrational modes. The observed and calculated vibrational frequencies are found to be in good agreement. Energy gap of the molecule was determined using HOMO and LUMO calculation. The gap value of 3.58 eV obtained by DFT/B3LYP show this structure is more stable in the gas phase. All calculations in this work were performed using the Gaussian 03 W software package.

Key words: Thiazole, Theoretical calculations, Spectroscopy, HOMO-LUMO.

PO 74

Ab-initio study of half-metallic ferromagnetism in the XC₂Sr (X = C, Si, Ge, and Sn) half-Heusler compounds

H. Rozale*, A. Amar*, A. Lakdja*, A. Chahed* and A. Sayede**

*Condensed Matter and sustainable development Laboratory (LMCDD), University of Sidi Bel-Abbes, Sidi
Bel-Abbes 22000, Algeria

**UCCS, CNRS-UMR 8181, Université d'Artois, Faculté des Sciences Jean Perrin, Rue Jean Souvraz, SP
18, 62307 Lens Cedex, France

hrozale@yahoo.fr

Abstract:

This In search of half-metallic ferromagnetism, we have studied the electronic structure and magnetic properties based on density functional theory (DFT) within the generalized gradient approximation (GGA) and GGA plus modified Becke and Johnson as the exchange correlation for XC₂Sr (X = C, Si, Ge, and Sn) half-Heusler compounds. The strong spin polarization of *p* orbital for C, Si, Ge, and Sn atoms is found to be the origin of ferromagnetic for all compounds leading to a total magnetic moment 1 μ_B .

Key words: Density functional theory; Half-Heusler compounds; Half-metallic ferromagnetic.

PO 75

First-principles prediction of structural, elastic, electronic and thermodynamic properties of the cubic SrUO₃-Perovskite

B. Sahli^{*/***}, H. Bouafia^{**}, B. Abidri^{***}, S. Hiadsi^{**}, N. Benkhattou^{***} and D. Rached^{***}

** Laboratoire de Génie Physique. Université IBN KHALDOUN .TIARET,14000, Algérie.*

sahli_belgacem@yahoo.fr

*** Laboratoire de Microscope Electronique ET Sciences des Matériaux, Université des Sciences ET de la Technologie Mohamed Boudiaf, département de Génie Physique, BP1505 El m'naouar, Oran, Algérie*

hamza.tssm@gmail.com

said.hiadsi@gmail.com.

**** Laboratoire des Matériaux Magnétiques, Université Djillali Liabés, Sidi Bel-Abbes 22000, Algérie.*

b_abidri@hotmail.com

nordine_bt@yahoo.com

rachdj@yahoo.fr

Abstract:

Bulk properties such as lattice constant, cohesive energy, total energy, bulk modulus and its pressure derivative of the cubic SrUO₃-Perovskite are predicted in their nonmagnetic (NM), antiferromagnetic (AFM) and ferromagnetic (FM) states using All-electron self consistent Full Potential Augmented Plane Waves plus local orbital (FP-(L)APW+lo) method within PBEsol Generalized Gradient density approximations. Our calculation allowed us to predict that the more stable magnetic state of the cubic SrUO₃-Perovskite is that of the ferromagnetic (FM). This work is the first prediction of elastic constants and their related parameters (Young modulus, shear modulus, Poisson ratio, Zener anisotropy and The Debye temperature) for this cubic compound using Mehl method. We have employed the GGA(PBEsol) and GGA(PBEsol)+U to investigate the electronic band structure, density of states and electronic charge density of SrUO₃-Perovskite. This part of this work shows that this material is a metal and this is due to the position of the Fermi energy in the conduction band. The charge density plot for [110] direction indicates that there is a strong ionic character along the Sr–O bond while the U–O bond has strong covalent character.

Finally, we have analyzed the thermodynamic properties using the quasi-harmonic Debye model to complete the fundamental characterization of cubic SrUO₃-Perovskite.

Key words: Perovskites; DFT; FP-(L)APW+lo; GGA-PBEsol; GGA+U; Elastic constants ; thermodynamic properties.



PO 76

Modeling and simulation of electronic and optical properties of ZnO

H.I. Sari Hassoun, A.E. Merad and A. Zerga

Département de Physique théorique, Faculté des Sciences, Université de Tlemcen, BP 119, Tlemcen, 13000, Algeria

hibaa.imane@yahoo.fr

a_zerga@yahoo.fr

merad_a@yahoo.fr

Abstract:

In this study We present the results of an ab-initio theoretical study of the electronic structural and optical properties corrected by scissor of zinc oxide in wurtzite phase using an implementation of the FP method (L) APW in the framework of the density functional theory (DFT); the potential for exchange and correlation is treated within the generalized gradient approximation of the Engel-Vosko GGA-EV for the calculation of electronic and optical properties of ZnO. To validate our approach, we compare the results with those obtained using the generalized gradient approximation parameterized by Perdew, Burk and Emzerhop Perdew (GGA-PBE). The frequency dependent complex dielectric function $\epsilon(\omega)$ is calculated as well as the reflectivity and absorption coefficient. Our calculations show that the optical absorption edge to $\epsilon_{xx}(\omega)$ and $\epsilon_{zz}(\omega)$ are located around 3.19 eV. The structural properties, the band structure and density of states are present. The lattice constants of ZnO calculated in this study are in agreement with the experimental values and the band gap obtained by the GGA-EV yielded a broad and narrow valence band relative to GGA-PBE. Moreover, EV-GGA yielded a large separation between the states d of Zn and states p of O, thereby reducing the repulsion p-d and therefore improved the energy band.

Key words: The theory of density functional theory, the approach of pseudo-potential, electronic properties, optical properties, ZnO.



PO 77

The thermodynamic properties and bonding feature of the some B2 rare-earth intermetallic compounds: Ab initio study

Abdessamad Sekkal*, Abdelnour Benzair** and Ghouti Merad*

**Laboratoire d'Etude et Prédiction de Matériaux, Unité de Recherche Matériaux et Energies Renouvelables, Département de Physique, Faculté des Sciences, Université Abou Bekr Belkaid B.P 119, 13000 Tlemcen, Algérie.*

asamad2002@yahoo.fr

g_merad@mail.univ-tlemcen.dz

***Département de Physique, Faculté des sciences, Université Djillali Liabes. 22000 Sidi Bel Abbés, Algeria.*

abenzair@yahoo.fr

Abstract:

The full-potential linearized augmented plane wave (FP-LAPW) method has been employed within the generalized gradient approximation (GGA) to investigate the structural and thermo-elastic properties of some rare earth intermetallics such as YAg, YCu, HoCu, LaAg, LaZn, and LaMg compounds. The calculated ground state properties such as lattice constants, bulk modulus and elastic constants agree well with the experiment. For HoCu and LaZn compounds, the thermodynamic properties are predicted [1] via the quasi-harmonic Debye model, using to predict the low-temperature behavior of the crystal. For the first time, the numerical estimation of the thermal properties is performed for these compounds and still await experimental confirmations. In addition, the chemical bonding of these compounds has been investigated in the light of topological analysis approach based on the theory of atoms in molecules (AIM).

Key words: Intermetallic compounds; Ab-initio calculations; Electronic structure; Elastic properties; Thermal properties.



PO 78

A Potential Energy Distribution Investigation using Force Fields and Quantum Mechanics Methods of the Methylated Glucose and Xylose derivatives: a Comparative Study

Ilham Naoual Taleb-Mokhtari, Abbassia Lazreg and Majda Sekkal-Rahal

Laboratoire de Microscopie, Microanalyse de la matière et Spectroscopie Moléculaire (L2MSM),

Département de Chimie, Faculté des Sciences, Université Djillali Liabes, B.P. 89, 22000,

Sidi Bel Abbas, Algeria

il_taleb@yahoo.fr;

ablazreg@yahoo.fr

majsekkal@msn.com

Abstract:

The aim of this study is to compare the theoretical spectra obtained by the method of force fields and the method of quantum mechanics of the methyl- β -D-glucopyranoside hemihydrate and methyl- β -D-xylopyranoside compounds. The vibrational spectra of these molecules recorded in the 4000-500 cm^{-1} spectral region for the FT-IR spectra and in the 4000-20 cm^{-1} spectral range for the FT-Raman spectra are presented.

A normal coordinate analysis has been done using a modified Urey-Bradley-Shimanouchi force field. The theoretical spectra have been obtained after a tedious refinement of the force constants. Thus, on the basis of the obtained potential energy distribution, each observed band in IR and in Raman has been assigned to a vibrational mode.

The optimized geometric parameters, conformational analysis, frequencies and the corresponding vibrational assignments of these molecules are theoretically examined by means of the DFT method 6-31++G(d,p) basis set. Furthermore, reliable vibrational assignments have been made on the basis of potential energy distribution (PED). A visual representation of the shape of the vibrational modes provided by the Gauss-View graphical interface for GAUSSIAN programs has facilitated the assignment of the calculated wave numbers. Theoretical vibrational spectra of the compounds are interpreted by means of PEDs using the VEDA 4 program.

Finally, we could conclude that the vibrational frequencies and PED obtained by the force fields modes (modified UBSFF) and DFT methods reproduce the vibrational spectra with good agreements in regards to those observed in IR and Raman.

Keywords: Methyl- β -D-glucopyranoside hemihydrate; Methyl- β -D-xylopyranoside; Potential Energy Distribution, Vibrational Spectra.

PO 79**Atropisomerism in N-(2-ethylphenyl)-N'-(2-methylphenyl) thiourea: Theoretical study**

A.Touadjine*, A. Mostefai* A. Rahmouni* and S. Humbel**

* *Laboratoire de Modélisation et de Méthodes de Calculs- Centre Universitaire de Saida, B.P. 138, Cité En-Nasr-20002- Saida – Algérie.*

** *Institut des Sciences Moléculaires de Marseille, Campus St Jérôme -Aix-Marseille Université, 13013 Marseille – France*

Abstract:

β -cyclodextrin and its derivatives form inclusion complexes with different enantiomers of a wide variety of guest molecules. The main purpose of the present theoretical investigation is to help to predict the enantiodiscrimination of N-(2-ethylphenyl)-N'-(2-methylphenyl) thiourea. It should be noted that this compound present two atropisomers that can be experimentally [1] separated by inclusion within the cavity of the hydroxypropyl β -cyclodextrin. It therefore appeared of interest to study, in the first part, the model compound called 1,3-di-o-tolyl-2-thiourea. We were interested then in the identification of the possible conformers of this compound. All conformers were fully optimized at different levels of theory. The energies and relative energies of all possible conformers are evaluated and discussed. Our calculations showed, as expected, that the pi-stacking conformer with respect to other structure is the most stable. Indeed, this conformer is shown (Figure 1) to bear a π - π stacking interaction; the parallel-displaced aromatic rings are sufficiently close (3.503Å from center to center) to give rise to a favorable interaction. This distance is in agreement with typical pi-stacking and parallel-displaced geometries reported in the literature [2-3] which range between 3.5 and 4.0Å.

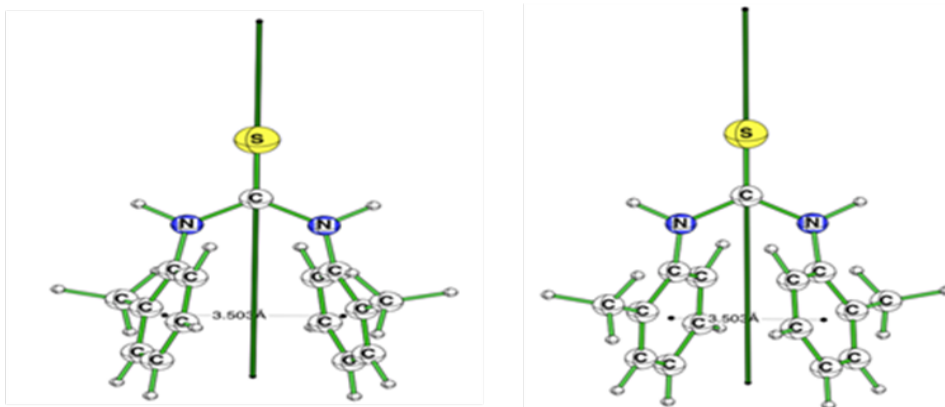


Figure.1 : Optimized structure of atropisomers of 1,3-di-o-tolyl-2-thiourea, using MP2/6-311G(d) level of theory.

Key words: Atropisomerism, hydroxypropyl β -cyclodextrin, pi-stacking conformer.

References:

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PO 80

Contribution to the study of AlGa_N/Ga_N high electron mobility transistors for biological applications

O. Zeggai, A. Ould-Abbas, H.Zeggai and M. Belarbi

*Research unit of Materials and Renewable energies (URMER), University Abou Bakr Belkaid, B.P. 119,
Tlemcen, Algeria*

zeggai_oussama@yahoo.com

Abstract:

Chemical sensors can be used to analyze a wide variety of environmental, biological gases and liquids. They may need to be able to selectively detect a target analyte. Different methods, including gas chromatography, chemiluminescence, selected ion flow tube, and mass spectroscopy, have been used to measure biomarkers. A promising sensing technology utilizes AlGa_N/Ga_N high electron mobility transistors (HEMTs). HEMT structures have been developed for use in microwave power amplifiers due to their high two dimensional electron gas (2DEG) mobility and saturation velocity. The conducting 2DEG channel of AlGa_N/Ga_N HEMTs is very close to the surface and extremely sensitive to adsorption of analytes. HEMT sensors can be used for detecting gases, ions, *pH* values, proteins, and DNA. In this work we review recent progress on functionalizing the surface of HEMTs for specific detection of glucose.

Key words: Biosensor, HEMT, AlGa_N/Ga_N, 2DEG, Glucose.

PO 81

Theoretical study of organic photonic crystals

K. Zellagui, A. Dekhira and O. Ouamerali

Faculté de Chimie, Laboratoire de Chimie Théorique Computationnelle et Photonique,

USTHB, El Alia 16111 Bab Ezzouar, Alger, Algérie

kheirouzell@yahoo.fr, ouameralio@yahoo.fr

azedbox@gmail.com

Abstract:

Photonic crystals are a new class of periodic dielectric media that can provide novel ways to manipulate and control light. The use of organic materials (polymers) for the fabrication of photonic crystal is currently being actively investigated. They are an interesting platform material for photonic crystal applications due to their ability to self-assemble into a variety of 1D, 2D, and 3D periodic structures and the ability to selectively incorporate additives.

In this work, we have modeled and optically characterized two polymeric 1D photonic crystals: A PVK-CA structure, consisting in alternated stacks of polyvinyl-carbazole (PVK) and cellulose acetate (CA) as well as a structure of lamellar polystyrene - polyisoprene (PS-PI). Such multilayer stacks of materials, known also as Bragg stacks can be useful for various photonic and optoelectronic applications, including solar cell and laser DFBs and DBRs.

In order to predict the photonic properties of these structures, we have implemented two computational codes using the programming environment “Matlab”: a PWE-based code to determine the band diagrams and a TMM-based code to calculate the reflectance of the investigated structures.

Dealing with polymeric photonic crystals leads to few challenges to override. The primary challenge is to obtain the large domain sizes needed for the optical frequencies of interest, as well as production of sufficient dielectric contrast between domains that provides the ability to further tailor the optical properties. In polymers the refractive index mismatch is normally small compared with other layered structures such as inorganic dielectrics ($n_{PVK} = 1.68 / n_{CA} = 1.47$ and $n_{PS} = 1.59 / n_{PI} = 1.51$), but this limitation can be compensated by employing a large number of layers, as our calculations show.

Key words: Photonic crystals, polymeric 1D photonic crystals, PWE, TMM.

PO 82

The critical Binder cumulant for bond diluted Ising model on a square lattice

Ismail Zergoug, Mustapha Aouaichia and Rachid Bouamrane

Université d'Oran des Sciences et de la Technologie USTO-M, Algeria

zergoug.ismail@gmail.com

mta.aouaichia@yahoo.fr

bouamranerachid@hotmail.com

Abstract:

The critical Binder cumulant U^* of bond diluted Ising model on square lattice is studied using Monte Carlo techniques. We discuss the depends of the value of the critical cumulant and the value of the transition temperature T_c obtained from U^* for different probabilities of bond dilution p . The decrease of critical Binder cumulant U^* and the transition temperature T_c are shown toward the increase of the probability of bond diluted p .

Key words: Binder cumulant, Ising model, Monte Carlo, Phase transition.

PO 83

Optimization of geometric parameters from a solar furnace with optical fiber supply

Chafika Zidani and Boumediene Benyoucef

Unit of Research on Materials and Renewable Energies, University of Tlemcen, 13000, Algeria

czidani10@yahoo.fr

Abstract:

A theoretical study of the heat transfer process that takes place in a special solar furnace is presented. Taking into account the possibility of transport of concentrated solar energy using optical fibres, we predict what may be expected in solar furnaces making use of such fibres.

The aims of this study are to optimize the coupling of a paraboloidal dish, which concentrates direct solar irradiance with dual axes tracking component, and the optical fibre, which transmits concentrated solar energy.

We present the daily power obtained at the output of the optical fibre, the power supply is estimated to be 20 W at the end. Then we show that the energy transported is diffused until the enclosure then disperse inside it, this energy is absorbed by the receiver. Temperatures higher than 1500°K may be reached while maintaining very good efficiency. Such furnaces have the extra advantage of having temperature gradients which may be perfectly determined.

Key words: concentrated solar energy, optical fibre, solar lighting, solar furnace.



PO 84

Silicon effect on atomic oxygen adsorption on hafnium nitride surface

S. Zouambia and D. Hammoutène

LTMM, USTHB University, BP32 El Alia, 16111 Bab Ezzouar, Algiers, Algeria

zouambia_s@yahoo.fr

dhammoutene@yahoo.fr

Abstract:

As one of the ultra-high temperature ceramics (UHTC), hafnium nitride (HfN) is regarded as one of the leading candidates for aerospace, engines, plasma arc electrodes, cutting tools, furnace elements and hypersonic vehicles applications. This is due to the combination of its amazing properties such as extremely high melting point, high hardness and relatively good thermal shock resistance. However, HfN is unstable in oxidizing atmospheres especially at high temperatures, which limits its applications. Oxidation of UHTC usually occurs on surfaces at first.

To clarify the interactions between oxygen and the surfaces of transition metal nitride, researchers have done many experiments. They have found that there exists gaseous NO or NO₂. Then this gas is desorbed from the substrate.

The goal of this study is to investigate the adsorption of atomic oxygen on the HfN (001) surface within a first-principles framework.

Our computational models were based on the fastest Density Functional Theory (DFT), as implemented in the Cambridge Serial Total Energy Package (CASTEP). A plane-wave basis set and ultra-soft pseudopotentials are used to simulate the properties of surfaces and interfaces.

Keywords: Adsorption, Density functional theory calculation, Electronic structure, Hafnium nitride, Surface.

PO 85

Conformation of ι -carrabiose in the presence of lithium cation and the acid form by DFT Study

Zouaoui Rabah Mourad, Yousfi Nouredine and M. Sekkal-Rahal

Laboratoire L2MSM, Faculté des Sciences Exactes. Université Djillali Liabes de Sidi Bel Abbas,

B.P. 89. 22000 Sidi Bel Abbas. Algeria

crmamourad@yahoo.fr ; nordvp@gmail.com

majsekkal@msn.com

Abstract:

Carrageenans are linear sulfated polysaccharides occurring as cell wall constituents in red algae and are used as texturing agents in the food industry. Their skeleton is composed of D-galactopyranose connected by links alternately α (1 \rightarrow 3) and β (1 \rightarrow 4). galactopyranose. The objective of our study is mainly to explore the conformational space and identify conformations corresponding to the lowest energies taking into account the geometrical parameters, the dihedral angles of the glycosidic bond and the different orientations of the hydroxymethyl and hydroxyl groups present in their structures in the presence of lithium cation. To achieve this goal, the ab-initio methods were used in the study of the structures of carrageenan iota carrageenan especially in vacuum and in the solvent using the PCM implicit model, as well as their structural characterization. The main results showed a significant effect of the ion on the stability against carrageenan, followed by the conformation of the hydroxymethyl group does not seem to affect their stability.



Figure 1 : τ - carrabiose charged (-1) (compound I), τ neutral -carrabiose (Compound II)

Full optimization of isolated compounds

Table1: Values of Φ and Ψ dihedral angles ($^{\circ}$) and Energy (kcal / mol) after optimization of structures from:

Disaccharide	$\Phi(^{\circ})$	$\Psi(^{\circ})$	Energy (kcal/mol)
Compound I	-86,4	73,7	-1548677.932985
Compound II	-85,8	74,9	-1558150,326711

Keywords: α -carrabiose, DFT method, B3LYP, M062X, implicit solvent.



PO 86

VALIDATION DU MODÈLE THÉORIQUE AB₄ DE L'EAU POUR LES SIMULATIONS DES MACROMOLÉCULES BIOLOGIQUES

A. Zanoun¹, s. Beladjine^{1,2}, m. Amrani^{1,2} et g. Vergoten³

1. Laboratoire de Biomécanique Appliquée et Biomatériaux. ENP d'Oran, Algérie.

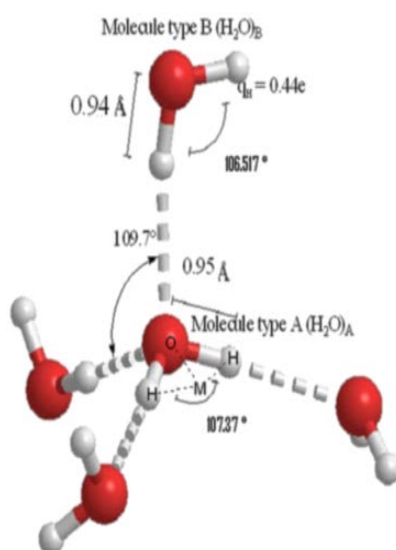
2. Faculté des Sciences Exactes, Université d'Oran, Algérie.

3. Unité de Glyco-biologie Structurale et Fonctionnelle, UST Lille, France

Résumé :

Il est important de modéliser avec précision les propriétés de l'eau pour bien simuler les macromolécules biologiques en milieu aqueux, Il existe plusieurs modèles (rigides, déformables ou polarisables). Le modèle géométrique AB₄ considère une architecture tétraédrique d'un cluster flexible composé d'une molécule centrale dite piégée de type A [(H₂O)_A] représentant 20% de l'échantillon et quatre autres molécules périphériques dites pièges de type B [(H₂O)_B] (80%) (voir Figure). Ce modèle prédit une pseudo- double structure de l'eau pour essayer d'expliquer pourquoi ce liquide est le solvant universel par excellence.

Afin de valider ce modèle, nous présentons dans cette étude à l'aide d'une étude par Dynamique moléculaire, l'influence des ions Na⁺ et Cl⁻ sur sa structure, ses caractéristiques et les liaisons hydrogènes. Les interactions intermoléculaires sont traitées par le potentiel SPC/E (Extended Simple Point Charge/). Des simulations de dynamique moléculaire ont été réalisées sur des solutions aqueuses de NaCl suivant une série de concentration dans les conditions ambiantes,





PO 87

Synthesis of phosphoenol pyruvate. Theoretical and experimental study

Amina Ghomri* and Abdelkrim Atmani**

* *École Préparatoire Sciences et Techniques Tlemcen, BP 165 RP Bel horizon ,13000 Tlemcen, Algerie*

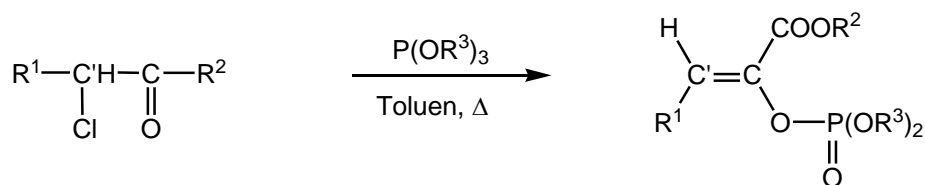
am_ghomri@mail.univ-tlemcen.dz

** *Département de Chimie, Faculté des Sciences, Université A. Belkaïd, B. P. 119, Tlemcen, 13000, Algérie*

ab_atmanii@yahoo.fr

Abstract:

A theoretical and experimental study of the reaction of α -chloropyruvate with trialkyl phosphites in toluene is reported . The phosphoenol pyruvate obtained were characterized by (^1H , ^{13}C and ^{31}P) NMR. DFT-based reactivity descriptors are used to explain the main reaction product found experimentally. Global and local reactivity indices namely global electrophilicity and Parr function were computed at B3LYP/6-311(d) level of theory. Solvent effect on the reactivity indices is elucidated. The computed regioselectivity is in good agreement with experimental outcomes.



Reaction of α -chloropyruvate with trialkylphosphites in Toluene.

Key words: α -chloropyruvate, phosphoenol pyruvate, electrophilicity index, regioselectivity, Parr function.

PO 88

Solvent effect on neutral form of iota carrabiose molecule : a DFT PCM study

N. Yousfi, C. Reguieg, Zouaoui Rabah Mourad and M. Sekkal-Rahal

Faculté des Sciences Exactes, Laboratoire L2MSM, Université Djillali Liabès de Sidi Bel Abbès, B.P.89,

Sidi Bel Abbès, 22000, Algeria

nordyp@gmail.com

Abstract:

Iota carrageenan is a sulfated linear polyosides largely used as a texturing agent for various applications in food, chemical, and pharmaceutical industries, this is due to its physical properties to form thermoreversible gels that are related to its conformation. The structure of one of the two repeating disaccharides constituting ι -carrageenan; the 4-O-sulfated- β -D-galactopyranosyl (1,4) 2-O-sulfated 3,6-anhydro- α -D-galactopyranose (see Fig. 1) is studied in this work.

During these two last decades, many works dealing with conformational studies of carbohydrates have appeared; most of them used classical methods to explore the structure of the conformers, such as molecular mechanics. More recently, a number of articles, using ab initio or density functional theory (DFT) studies, have begun to appear.

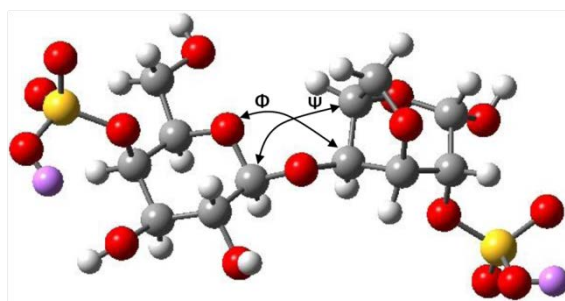


Figure 1: Structure of ι -carrabiose disaccharide, (neutral form), dihedral angles Φ and Ψ around the glycosidic linkage.

The B3LYP density functional was used with the 6-31G(d) basis set to perform relaxed energetic contour maps for the neutral form (with an alkali metal Li^+). Only one starting conformation has been considered to perform all the calculations. Rigid energetic maps have been then constructed either by addition of diffuse or polarization functions to the basis set obtaining in that way 6-311G(d)//6-31G(d), 6-311G(d,p)//6-31G(d) energetic maps that have been carefully examined.

The obtained structures corresponding to the lower energy conformers have been then fully optimized using different basis sets with the B3LYP method, a reversion in term of energy has been observed for some minima in the case of the neutral disaccharide in presence of solvent, this was attributed to the large grid of 30° that could lead to the exclusion of an intermediate value corresponding to the real minimum of energy. We thus suggest that after establishing potential energy maps it is essential to proceed to full optimizations of the lower energy conformers.

Key words: disaccharide, Density functional theory, α -carrabiose, potential energy maps, alkali metal Li^+

PO 89

Theoretical Study of the enantioselective reduction of prochiral ketones promoted by Amino Acid-Derived ruthenium Complexes

Yazid Meftah^{*}, Françoise Delbecq^{**} and Youcef Boumedjane^{*}

^{*} *Laboratoire de Chimie appliquée, Université Mohamed Khider, Biskra, BP 145, 07000, Algérie*

yazidmeftah@yahoo.fr

yboumedjane@yahoo.fr

^{**} *Laboratoire de Chimie, Ecole Normale Supérieure, 46 allée d'Italie, 69364 Lyon Cedex 07, France*

F.delbecq@ens-lyon.fr

Abstract:

Recently, a proline-amide has been experimentally employed as an effective chiral catalytic precursor in the ruthenium-mediated asymmetric reduction of prochiral ketones to produce the corresponding secondary alcohols, in this work we suggest a mechanism for this reduction process, the full free energy profile for the transfer hydrogenation is calculated according to the outer-sphere reaction mechanism. Two factors are demonstrated to influence the stereoselectivity of the process, the energy difference between the intermediate hydrogenated catalyst, and the existence of a stabilizing CH- π interaction between the (p-cymene) ligand of the catalyst and the phenyl moiety of the substrate. Further calculations show that inclusion of dispersion interactions (using the B3LYP-D2 correction or the M06 functional) has no great influence for reproducing the enantioselectivity.

Key words: asymmetric transfer hydrogenation- DFT-enantioselectivity-ruthenium.

PO 90

Origin of ferromagnetism in the half-Heusler XRbCs compounds (X=N, P and As)

Mohammedi Mohammed Walid, Rozale Habib and Hamdad Noura

Condensed Matter and Sustainable Development Laboratory, University of Sidi Bel-Abbes, Sidi Bel-Abbes 22000, Algeria

Abstract –

The magnetic properties arise from the electronic states at the Fermi level in one spin channel, which induce a high spin polarized current. Transition metals have been widely studied in this area due to localized d-electrons of a partially filled atomic shell. Spin-polarization in systems without transition metals attracts increasing research interest as potential materials in spintronic devices. However, materials based on alkali and alkaline earth metals show half-metallicity (HM) where the magnetic order is carried out by the p states. Among this new class of materials, namely d⁰-HM ferromagnets, alkali and alkaline earth metals with VI-elements were found to be HM ferromagnets with a total polarization of holes. In the present paper, we focused on the hypothetical half-Heusler compounds XRbCs, where X denotes N, P and As. We expect that these materials exhibit half-metallicity from the polarization of p-electrons of IV-elements. By the use of the first-principles approach, we investigate the magnetic properties related to the electronic structure. A density functional theory was used to study the origin of ferromagnetism in the half-Heusler XRbCs compounds (where X=N, P and As). The results predict a stable atomic arrangement with a ferromagnetic order. The spin-polarized calculations give a total magnetic moment of about 1μB. The most important property in these hypothetical compounds is that the half-metallicity is originated from the polarization of the p-orbitals originated from N, P, and As atoms. We also find that the half-metallicity is maintained on a wide range of lattice constants and therefore offers the possibility to grow such materials on various semiconductor substrates. This new Half-Heusler family alloy can be proved as an ideal candidate for spin valves and magnetic tunnel junction applications (MTJs).

Keywords – Half-Heusler compound, Alkali metal, Ferromagnetism, Density functional theory.

PO 91

Calculation of High Field Electron Transport Properties in 6H-SiC Using Monte Carlo Simulation: 3 and 5-valley models

Nora Talha, Abd-Ed-Daim Kadoun

*L2MSM laboratory - Physics Department- Faculty of Exact Sciences
Djilali Liabes University. 22000. Sidi Bel-Abbes. Algeria*

Physique_sc@yahoo.fr

akadoun@yahoo.com

Abstract:

Owing to the flexibility of the method, the simplicity of its principle, and the relative ease of its implementation, Monte Carlo simulation is widely used as a powerful tool for the study of the physical working of materials and related electronic components. In addition, it can be made as rigorous as we want. Amongst the numerous SiC polytypes, 6H-SiC is believed to be the most important one for device fabrication technology, due to its easiest preparation and its high conduction band offset with SiO₂. We present here the stationary results obtained by Monte Carlo calculations, showing the influence of the temperature and the doping concentration on the electron drift velocity, energy and mobility in 6H-SiC semiconductor when an electric field is applied in the perpendicular direction to the c axis. However, when a high electric field is applied, more than one conduction band valley is expected to be involved in the electron transport. The Monte Carlo method used to characterize SiC material is based on two nonparabolic models implementing three valleys and five valleys respectively and takes into account scattering mechanisms such as acoustic and polar optical phonons, intervalley diffusion and electron-impurity collisions. Comparisons are made between the two and three-valley models.

Key words: SiC, Band structure, Scattering, Monte Carlo calculation, Electron transport.



PO 92

Study of bgan materials grown on aln/sapphire by movpe

M. Bouchaour^{*1}, N. Maloufi³, G. Orsal^{2,4}, S. Gautier^{2,4}, A. Ould-Abbas¹, N.E. Chabane Sari¹, A. Ougazzaden⁵

1. Unité de Recherche Matériaux et Energies Renouvelables (URMER) – Université Abou Bekr Belkaid - Tlemcen, BP 119 Tlemcen, Algérie.

*Bouchaour.m@gmail.com

2. Laboratoire Matériaux Optiques, Photonique et Systèmes, Université de Metz and SUPELEC, 2 rue E. Belin 57070 METZ, France.

3. Laboratoire d'Etude des microstructures et de mécanique des matériaux UMR CNRS 7239 Ile du Saulcy 57045 METZ cedex 1, France.

4. UMI 2958 Georgia Tech-CNRS.

5. Georgia Institute of technology / GTL 2-3 rue Marconi 57070 Metz, France. UMI 2958 Georgia Tech-CNRS

Abstract:

GaN and related alloys (GaAlN, InAlN, InGaN) are ideal candidates for light emitting diodes (LEDs), laser diodes operating throughout ultra violet to green visible spectral range and high frequency electronic devices. Their high thermal and chemical stability allow the devices to work safely under highly aggressive environments i.e. high temperature or high pressure. However one of the limiting aspects of GaN-based materials is their relatively poor crystal quality due to the necessity of heteroepitaxy. New boron based materials present the advantage to be lattice matched on Silicon Carbide (SiC) and Aluminium Nitride (AlN) with 8% and 17 % respectively.

In this study, we report the results of morphological and structural properties of BGaN films grown on AlN/sapphire in T-shaped MOVPE reactor for different thicknesses. We find that single crystal of $B_xGa_{1-x}N$ can be produced up to a given amount composition x depending on the thickness of the layers and x is higher than the theoretical predictions. This parameter (the thickness deposited) is in relation with the strain elastic energy accumulated.

Key words: BGaN, AFM, SEM, XRD, TEB/III, Thickness, boron composition, MOVPE

PO 93

Methods of quantum chemistry applied to the conformational study of Nu (v) caragreenan.

Okkacha Hamhami* · Abdelkader M. El Horri , and Majda Sekkal-Rahal ***

L2MSM laboratory - Faculty of Exact Sciences

Djilali Liabes University. 22000. Sidi Bel-Abbes. Algeria

okkacha.hamhami@yahoo.fr

a.melhorri@yahoo.fr

majsekkal@msn.com

Abstract:

Carrageenan is the generic name for a family of natural, water-soluble sulfated galactans extracted from numerous species of red seaweeds. the objective of this study is to investigate the structural characteristics of complex organic molecules such as carrageenan, to establish a relationship between energy and the structure of the disaccharide, that is to say, to determine all conformations corresponding to the lowest energy. We were interested in this study on the effect of the orientations of the various sulfate groups . In this research we studied on the structure and rate of levels of energy by using DFT methods in the level of B3LYP/6-31+G**,

Key words: Carrageenan, DFT, Nu (v) caragreenan, Quantum Mechanics

Fig. 1. chemical structure of Nu (v) carrageenan

List of Participants

Oral communications

Nr.	Name	Communication title	Country
01	Reinhold F. Fink	<i>Applying Computational Chemistry on Material Properties in Organic Electronic Devices</i>	Germany
02	Hyungjun Kim and Yoon Sup Lee	<i>Protocols to Calculate Redox Potentials of Transition Metal Complex Ions</i>	Korea
03	Henning Hopf	<i>Aromatic Chemistry 150 Years after Kekulé: From the Plane to Three-dimensional Space</i>	Germany
04	Karin Fink	<i>Transition metal compounds in magnetism and catalysis</i>	Germany
05	Lotfi Belkhiri	<i>Relativistic computational study of highly selective N-ligands for lanthanides(III)/actinides(III) separation</i>	Algeria
06	Gérard Vergoten	<i>A Cybernetic Approach to Molecules, Molecular Recognition and Chemical Communication</i>	France
07	Aurélien Moncomble	<i>Elucidation of metal complex structures by TD-DFT calculations coupled with electronic spectroscopies</i>	France
08	Dalila Hammoutene	<i>Computational Molecular Design of Nonlinear Optical Materials</i>	Algeria
09	Sahar Abdalla	<i>Isolated and Deposited Potassium Clusters</i>	Sudan
10	Marwan S. Mousa	<i>Microwave Harmonics Generated in Laser-Assisted Scanning Tunneling Microscopy – Their Significance Regarding Terahertz Sources in Laser Assisted Field Emission</i>	Jordan
11	A. Aboulmouhajir	<i>Molecular modeling petro chemistry and therapeutic chemistry</i>	Morocco
12	Lounis Mourad	<i>Crash energy dissipation in the head security helmet</i>	Algeria

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13	M. Ellouze	<i>Critical behavior in manganites in $\text{La}_{0.67}\text{Ba}_{0.22}\text{Sr}_{0.11}\text{Mn}_{1-x}\text{Fe}_x\text{O}_3$ ($0 \leq x \leq 0,2$)</i>	Tunisia
14	Hans-Heinrich Limbach	<i>NMR Studies of acid-base interactions: from hydrogen bonded model systems to proteins</i>	Germany
15	Hossein Eslami	<i>Molecular Dynamics Simulation of a Polyamide- Nanotube Nanocomposite</i>	Iran
16	Mohammad El- khateeb	<i>Organoiron Selenocarboxylate Complexes: Synthesis, characterization and Reactivity</i>	Jordan
17	Cenk Selçuki	<i>Molecular Modeling of Metal Ion Interactions with Biochemical Molecules</i>	Turkey
18	Alberto Del Rio	<i>Computational design of epigenetic drugs: past, present and future</i>	Italy
19	Abdelkader Souifi		
20	Ashraf H. Abadi	<i>Mining ZINC Database to Discover Potential Phosphodiesterase 9 Inhibitors Using Structure-Based Drug Design Approach</i>	Jordan
21	Saber Chatti	<i>Synthesis and characterization of polymers from biosourced monomers</i>	France
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25	Sidi Mohamed Mekelleche	<i>Theoretical study of the mechanism, regio- and stereo-selectivity of cycloaddition reactions</i>	Algeria
26	A. Sayede	<i>Insight on the ferroelectric properties in $(\text{BiFeO}_3)_2(\text{SrTiO}_3)_4$ superlattice: from experiment and ab initio calculations</i>	France

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28	<i>Yaseen A. Al-Soud</i>	<i>Synthesis and Biological Evaluation of Phenyl Substituted 1H-1, 2, 4-Triazoles as Non-Steroidal Inhibitors</i>	<i>Jordan</i>
29	<i>Faouzi Lakrad</i>	<i>Nonlinear Vibrations in Atomic Force Microscopy Systems</i>	<i>Morocco</i>
30	<i>Ahmad Telfah</i>	<i>Online Nuclear Magnetic Resonance (NMR) detection of mass and volume limited living cancer cell and other biological samples</i>	<i>Germany</i>
31	<i>Samir EL Zein</i>	<i>Stock markets simulations: from maths to clients</i>	<i>Lebanon</i>
32	<i>Isamail Trabelsi</i>	<i>Co-pyrolysis of landfill leachate reverses osmosis concentrate with sewage sludge in a fixed-bed reactor</i>	<i>Tunisia</i>
33	<i>Maged Mohammed</i>		<i>Egypt</i>
34	<i>Nasser Chellouah</i>	<i>Calcined clay in the futur cement</i>	<i>Algeria</i>
35	<i>Mostefa Belkhatir</i>	<i>Laboratory Study on Static Liquefaction of Overconsolidated Silty Sand Soils: Effect of Sample Preparation</i>	<i>Algeria</i>



Poster presentations

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PO 01	I.Abdelli	<i>Study of the Interaction β-Secretase-Flavonoids by The Molecular Modeling Methods: The Future Treatment of Alzheimer Disease</i>	Algeria (Tlemcen)
PO 02	K.Adji	<i>Structures and Properties of Indigo N-Glycosides</i>	Algeria (Sidi Bel Abbès)
PO 03	N.E-.Y. Amraoui	<i>DFT Study of Nucleic Acid Base Pairs Complexes</i>	Algeria (Algiers)
PO 04	Macho Anani	<i>Ni/SiC-6H Schottky diode for a very sensitive air-pollution detection</i>	Algeria (Sidi Bel Abbès)
PO 05	T. Ardjani	<i>Theoretical Study of the Structure and ¹H and ¹³C NMR Spectrums of Glutaconaldehyde Stereoisomers</i>	Algeria (Tlemcen)
PO 06	F. Azza	<i>Calculation of cross sections by an optical potential method in ESEM: Monatomic gases case</i>	Algeria (Sidi Bel Abbès)
PO 07	K. Babesse	<i>Structural, electronic and optical properties of BaX (X=S and Te) alloys</i>	Algeria (Algiers)
PO 08	B. Bahloul	<i>Ab initio calculations of structural, electronic and thermodynamic properties of BaSrTe alloys</i>	Algeria (Algiers)
PO 09	Bakhouché Kahina	<i>Structural and spectroscopic properties of a complex of vitamin E with vanadyl (II): Insight from ONIOM study</i>	Algeria (Algiers)
PO 10	R. Becharef	<i>Study of MIM structures for HF detection</i>	Algeria (Sidi Bel Abbès)
PO 11	A. Bedia	<i>Comparative Morphology, Structure and Optical Properties of Al, Cu and Sn Doped ZnO Nanostructure Synthesized by Spray Pyrolysis</i>	Algeria (Tlemcen)
PO 12	F. Z. Bedia	<i>Growth and Characterization of Tin Doped Zn Oxide Thin Films</i>	Algeria (Tlemcen)
PO 13	A. Bekhti-Siad	<i>THEORETICAL STUDY OF 3D TRANSITION METAL/GERMANIUM COMPOUNDS</i>	Algeria (Mascara)
PO 14	Bekhti-Bensalem.N	<i>Application of docking methodologies for the discovery of novel tumor cell migration inhibitors</i>	Algeria (Sidi Bel Abbès)
PO 15	L. Bekri	<i>Conformational characteristics of alginates and their interaction with the sodium ions: study by DFT</i>	Algeria (Sidi Bel Abbès)
PO 16	M. Belarbi	<i>Modeling of the electrical parameters of a dye-sensitized solar cell</i>	Algeria (Tlemcen)
PO 17	Khadidja Bellifa	<i>Estimation of the Acute Toxicity of Halogenated Phenols using Semi-empirical Quantum Chemistry Methods</i>	Algeria (Tlemcen)
PO 18	M.K. Benabadji	<i>Structural and mechanical properties of YM2 (M:Ni, Cu, Zn) Laves phases studied by first-principles calculations</i>	Algeria (Tlemcen)

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PO 20	B. Benbahi	Study of structural, elastic and electronic properties of TbX (X=N, P, As, Sb) compounds using LSDA and LSDA+U approach.	Algeria (Oran)
PO 21	Wafaa Benchouk	Regio- and Diastereoselectivity of the 1,3-Dipolar Cycloaddition of α -aryl Nitron with Methacrolein. A Theoretical Investigation	Algeria (Tlemcen)
PO 22	M. Benkabou	Electronic and mechanical properties of the fluoroperovskite LiBeF ₃	Algeria (Sidi Bel Abbès)
PO 23	Mohamed El Amine Benmalti	Theoretical study and Born Oppenheimer Molecular Dynamics calculation of the ν O-H IR Spectra for Acetic Acid Cyclic Dimers	Algeria (Mostaganem)
PO 24	N.E. Houda. Benmansour	Discretization of continuum states. Application to the atomic excitation	Algeria (Tlemcen)
PO 25	Amel Benmouna	Polymer based photovoltaic solar cells: Prospects and challenges	Algeria (Tlemcen)
PO 26	A. Ben Rhaïem	Electric and dielectric studies of the [N(CH ₃) ₃ H] ₂ CuCl ₄ compound at low temperature	Tunisia (Sfax)
PO 27	Nour el Houda. Bensiradj	Theoretical study of the clusters (ZnO) ₆ substituted by tellurium atoms	Algeria (Algiers)
PO 28	N. Bestaoui-Berrekhi-Berrahma	DFT AND MP2 CONFORMATIONAL STUDY OF 3, 6 ANHYDRO- α -D-GALACTOSE MOLECULE IN GAS PHASE AND IN WATER	Algeria (Sidi Bel Abbès)
PO 29	A. Bouabça	Structural, electronic, and magnetic properties of RbSrX (X=C, Si, Ge) half-Heusler	Algeria (Sidi Bel Abbès)
PO 30	N. Bouarra	Bioconcentration factor of PolyChloroBiphenyl in the environment: modeling and QSPR study	Algeria (Annaba)
PO 31	Sonia Boumendil	Influence of the used solvation model on the computation of electronic spectra of metal complexes: the example of Al(III)-caffeic acid system	Algeria (Sidi Bel Abbès)
PO 32	A. Boutasta	Ab initio analysis of the conformations of Acetylcholine	Algeria (Tlemcen)
PO 33	Z. Bouzid	Estimation of solar radiation and sizing method for autonomous photovoltaic system. Application to the west of Algeria	Algeria (Tlemcen)
PO 34	Yamina Bouzidi	A DFT Relativistic Study of Cyanide [MN ³ (CN) ₂] ²⁻ and Isocyanide [MN ³ (NC) ₂] ²⁻ (M ³⁺ = Ce, U; N ³⁻ = N(SiMe ₃) ₂) Complexes.	Algeria (Constantine)
PO 35	Chahed Abbes	Ab-initio calculations of the electronic structure and the magnetic properties of perovskite ruthenate CaRuO ₃ : Good candidate for the fabrication of superconducting multilayers	Algeria (Sidi Bel Abbès)
PO 36	Hafida Chemouri	Theoretical Explanation of the Effect of 1-ethylpyridinium Trifluoroacetate Ionic Liquid in the Promotion of Diels-Alder Reactions of Isoprene with acrylic acid	Algeria (Tlemcen)

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PO 38	Ismail Daoud	<i>Molecular modeling evaluation of novel piperazine derivatives of flavones as potent anti-inflammatory agent</i>	Algeria (Tlemcen)
PO 39	S. N. Derrar	<i>Theoretical Study on Some Unnatural Amino Acids Used as Probing Molecules in Nonlinear Optics</i>	Algeria (Sidi Bel Abbès)
PO 40	A.Djedouani	<i>Synthesis Structures, catecholase activité and Theoretical study of Schiff bases derivatives from DHA</i>	Algeria (Constantine)
PO 41	F. Djilali-Kobibi	<i>Study of the transfer of charge in the molecules combined by the methods of quantum chemistry</i>	Algeria (Sidi Bel Abbès)
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PO 44	Amina Fezazi	Interaction of iota- and kappa-carrabiose with monovalent cations studied by DFT	Algeria (Sidi Bel Abbès)
PO 45	Filali Sihem	New theoretical investigation on the electronic structure and magnetic interaction for both perovskites cubic SrFeO_3 and CaFeO_3 oxides	Algeria (Sidi Bel Abbès)
PO 46	R. Fodil	On the importance of the BSSE-CP correction during optimization of κ -carrabiose-water complexes	Algeria (Sidi Bel Abbès)
PO 47	Gheriballah Slimane	Half-metallicity in the half-Heusler RbSrX compounds ($X = \text{C, Si, Ge}$)	Algeria (Sidi Bel Abbès)
PO 48	Mahfoud Hadj-benali	The Dipole Moment, Polarizabilities, and First Hyperpolarizabilities of D/A Metal Porphyrins. A Comparative and Computational Study	Algeria (Algiers)
PO 49	Djebar Hadji	Theoretical study of structural and nonlinear optical properties of cyclic phosphazenes	Algeria (Saida)
PO 50	Hafsi Zoulikha	Gas effect on the emission of backscattered electrons in an HPSEM	Algeria (Sidi Bel Abbès)
PO 51	Hallouch Mustapha	Study by molecular modeling opportunities adsorption of Desethyl-s-Atrazine and Desisopropyl Atrazine on montmorillonte	Algeria (Sidi Bel Abbès)
PO 52	Harkati Dalal	Structure and physical-chemistry property relationship for indole derivatives	Algeria (Biskra)
PO 53	Yamina Harnane	On natural convection in an open geometry	Algeria (Oum-El-Bouaghi)
PO 54	Johnny Henderson	Higher Order Boundary Valued Problem for Impulsive Differential Inclusions	USA (Texas)
PO 55	A. Dekhira	FDTD Modeling of Silicon-based Photonic Crystals	Algeria (Algiers)
PO 56	Kerassa Aicha	Lipophilic efficiency Analysis and Comparison of Drug Efficacy of Triazolothiadiazole Derivatives by QSAR Analysis	Algeria (Biskra)
PO 57	M. Khalfa	Ab Initio Study of Structural, Elastic, electronic and thermal Properties of Full Heusler Compounds Fe_2VX ($X = \text{Al, Ga}$)	Algeria (Algiers)
PO 58	A. Kourdassi	FP-LMTO calculations of the structural, elastic, thermodynamic and electronic properties of the ideal-cubic perovskite BiGaO_3	Algeria (Sidi Bel Abbès)
PO 59	Lafifi Ismahan	Theoretical studies on histamine tautomerism	Algeria (Guelma)
PO 60	Abdelaziz Lakdja	Origin of magnetism in the sp-half metallic compounds	Algeria (Sidi Bel Abbès)

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PO 62	Abbassia Lazreg	<i>Conformational and Vibrational Study in the Gas Phase of some Amino Acids: Cysteine, Serine and Aspartic Acid</i>	Algeria (Sidi Bel Abbès)
PO 63	M. A. Mahi	<i>A DFT study of the Regio- and Stereoselectivity of the Aza Intramolecular-Diels-Alder reaction yielding to the formation of the 5aH-chromeno [2,3-c]acridine</i>	Algeria (Tlemcen)
PO 64	Imane Mammar	<i>Existence results for prion diseases model</i>	Algeria (Sidi Bel Abbès)
PO 65	N. Massout	<i>DFT study of the degradation mechanism of the anticancer drug imexon in aqueous solution</i>	Algeria (Algiers)
PO 66	N. Meçabih	<i>Conformational analysis of l-carrabiose tg using semiempirical methods</i>	Algeria (Sidi Bel Abbès)
PO 67	A. Merouane	<i>A DFT study of the Halogenation reaction in glutaconaldehyde benzoyl ester: Application of the static approaches of the chemical reactivity</i>	Algeria (Saida)
PO 68	Samir Meskaldji	<i>Magnetic exchange coupling in MII2 U(IV) Complexes (M= Cu, Zn). A relativistic DFT study.</i>	Algeria (Constantine)
PO 69	B. Messaoudi	<i>A CBS Study of 1-butene Reaction with Triplet Oxygen Atom O (³P)</i>	Algeria (Tlemcen)
PO 70	Moulay Nouredine	<i>Predictive study of physical properties of new multiferroic materials type ABO₃</i>	Algeria (Sidi Bel Abbès)
PO 71	Hidayet Moulessehoul	<i>C-Mannosylation and O-Fucosylation</i>	Algeria (Sidi Bel Abbès)
PO 72	B.Ouari	<i>Influence of the magnetization damping on Magnetic Susceptibility and Dynamics Hysteresis loops of biaxial nanoparticle</i>	Algeria (Tlemcen)
PO 73	R. Rahmani	<i>Molecular structure, Vibrational frequencies and frontier molecular orbital calculations on C₂₀H₁₅S₃N₂O₂F compound using Hartree Fock and Density Functional Theory</i>	Algeria (Mostaganem)
PO 74	H. Rozale	<i>Ab-initio study of half-metallic ferromagnetism in the XC₂Sr (X = C, Si, Ge, and Sn) half-Heusler compounds</i>	Algeria (Sidi Bel Abbès)
PO 75	B. Sahli	<i>First-principles prediction of structural, elastic, electronic and thermodynamic properties of the cubic SrUO₃-Perovskite</i>	Algeria (Tiaret)
PO 76	H.I. Sari Hassoun	<i>Modeling and simulation of electronic and optical properties of ZnO</i>	Algeria (Tlemcen)
PO 77	Abdessamad Sekkal	<i>The thermodynamic properties and bonding feature of the some B2 rare-earth intermetallic compounds: Ab initio study</i>	Algeria (Tlemcen)
PO 78	Ilham Naoual Taleb-Mokhtari	<i>A Potential Energy Distribution Investigation using Force Fields and Quantum Mechanics Methods of the Methylated Glucose and Xylose derivatives: a Comparative Study</i>	Algeria (Sidi Bel Abbès)

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PO 79	A.Touadjine	<i>Atropisomerism in N-(2-ethylphenyl)-N'-(2-methylphenyl) thiourea: Theoretical study</i>	Algeria (Saida)
PO 80	O. Zeggai	<i>Contribution to the study of AlGaN/GaN high electron mobility transistors for biological applications</i>	Algeria (Tlemcen)
PO 81	K. Zellagui	<i>Theoretical study of organic photonic crystals</i>	Algeria (Algiers)
PO 82	Ismail Zergoug	<i>The critical Binder cumulant for bond diluted Ising model on a square lattice</i>	Algeria (Oran)
PO 83	Chafika Zidani	<i>Optimization of geometric parameters from a solar furnace with optical fiber supply</i>	Algeria (Tlemcen)
PO 84	S. Zouambia	<i>Silicon effect on atomic oxygen adsorption on hafnium nitride surface</i>	Algeria (Algiers)
PO 85	Zouaoui Rabah Mourad	<i>Conformation of α-carrabiose in the presence of lithium cation and the acid form by DFT Study</i>	Algeria (Sidi Bel Abbès)
PO 86	A. Zanoun	<i>Validation du modèle théorique ab4 de l'eau pour les simulations des macromolécules biologiques</i>	Algeria (Oran)
PO 87	Amina Ghomri	<i>Synthesis of phosphoenol pyruvate. Theoretical and experimental study</i>	Algeria (Tlemcen)
PO 88	N. Yousfi	<i>Solvent effect on neutral form of iota carrabiose molecule : a DFT PCM study</i>	Algeria (Sidi Bel Abbès)
PO 89	Yazid Meftah	<i>Theoretical Study of the enantioselective reduction of prochiral ketones promoted by Amino Acid-Derived ruthenium Complexes</i>	Algeria (Biskra)
PO 90	Mohammedi Mohammed Walid	<i>Origin of ferromagnetism in the half-Heusler XRbCs compounds (X=N, P and As)</i>	Algeria (Sidi Bel Abbès)
PO 91	Nora Talha	<i>Calculation of High Field Electron Transport Properties in 6H-SiC Using Monte Carlo Simulation: 3 and 5-valley models</i>	Algeria (Sidi Bel Abbès)
PO 92	M. Bouchaour	<i>STUDY OF BGaN MATERIALS GROWN ON AlN/SAPPHIRE BY MOVPE</i>	Algeria (Tlemcen)
PO 93	Okkacha Hamhami	<i>Methods of quantum chemistry applied to the conformational study of Nu (v) caragreenan</i>	Algeria (Sidi Bel Abbès)