7th African School on Electronic Structure Methods and Applications - ASESMA 2023 | (SMR 3847)

12 Jun 2023 - 23 Jun 2023
Outside, Kigali, Rwanda

P01 - AGENA Agegnehu Abezu

Theoretical investigations of superconducting properties of Hydrogen Sulfide

P02 - AMADOU Nourou

Dynamic response of single-crystal iron from shock compression to spall fracture using molecular dynamics simulations

P03 - BAKASA Namarome Carolyne

Time-Dependent Density Functional Theory calculations will evaluate the photosensitizer's chemical properties and Molecular Dynamics simulation will predict the interaction mechanism between the photosensitizers and the microbes. Photodynamic antimicrobial chemotherapy effectiveness will experimentally and theoreticall tested on E. coli and S. aureus using the synthesized porphyrin and metalloporphyrins photosensitizers.

P04 - BALOI Mmapula

Structural, Magnetic, and Thermoelectric Properties of GdRuSi Half-Heusler Compound: A Density Functional Theory (DFT) Study

P05 - BOUKACHABIA Samira

DFT study on Pb substitution in all ignorganic-perovskites

P06 - DON-TSA Delchere

Below is my abstract

P07 - ELSAYED Wala

Dirac plasmon in novel topological semimetals: insights from ab-initio calculations

P08 - FWALO Chewe

First principles study of defects in the wide band gap 2 dimensional materials high performance Li-ion and Na-ion anode batteries applications.

P09 - HUSSIEN A. M. Musa

First-Principles Insights into Electric-Field Induced Phase Transition in Magnetic Tunnel Junctions

P10 - INNAN Nouhaila

Quantum Computing for Electronic Structure Calculations

P11 - JOLAYEMI Rita Omamuyovwi

Density-functional study of the thermodynamic properties and the pressure-temperature phase diagram of Mg_2SiO_4.

P12 - KEBEDE Damena Tadewos

Transition Metal Complexes for alternative drug synthesis as antibacterial and Antioxidant Activities: A Combined Experimental, DFT, and Molecular Docking Studies

P13 - KIRA Willy Bellard

The effect of pressure on electron-phonon interaction in metallic systems : case of MgB_2

P14 - KOTOKO Koudzo Jacques

Temperature-dependent mechanical properties of graphynes and applications: Machine Learning vs classical potential

P15 - MAKUNGU Patience

AB INITIO CALCULATIONS ON OPTOELECTRONICS PROPERTIES OF LEAD-FREE DOUBLE HALIDE (ELPASOLITE) PEROVSKITE Cs_2AgBiI_6

P16 - MULE Mumbi Gloria

STRUCTURAL AND ELECTRONIC PROPERTIES OF BULK MOLYBDENUM DISULFIDE: A DENSITY FUNCTIONAL THEORY STUDY

P17 - MUNYUKI Gadzikano

Enzyme encapsulation for carbon dioxide capture and conversion in Metal-Organic Frameworks.

P18 - ODHIAMBO Otieno Vincent

Investigation of Magnetic properties of FeMnPIn using GGA functionals

P19 - OKELLO Alex

Influence of the pH of anthocyanins on the efficiency of dye sensitized solar cells

P20 - OYENIYI Ezekiel

Electronic and optical properties of antiperovskites: The GW/BSE approach

P21 - PONRA Abraham

Density-Functional Theory Study of the Reactivity of Buckminsterfullerene towards Hydroxyl Radicals

P22 - SENE Pape

Stability, electronic and structural properties of aluminene from first-principles calculations

P23 - TAJOUO TELA Herve

Rovibrational states calculations of the H_2O – HCN heterodimer with the Multiconfiguration Time Dependent Hartree method.

P24 - TRIKI EP SALLAMI Mouna

Temperature dependence on the interband transition in single modified droplet epitaxy $GaAs/Al0.3Ga0.7As$ quantum dots

P25 - UTO Oghenekevwe Timothy Oghenekevwe

First principles study of Electronic, Structural, Phonon and Thermodynamic properties of XCrSb (X= Fe, Os) half-Heusler spintronic compounds

ABSTRACT

Pressure-stabilized hydrides are a new rapidly growing class of high-temperature superconductors which is believed to be described within the conventional phonon-mediated mechanism of coupling. Hydrogen, the lightest element in the periodic table, has been predicted to metalize under extreme compression. Metallic hydrogen is believed to be a room-temperature superconductor. Due to the considerable experimental challenges of reaching such a state, the material has often been deemed the holy grail of condensed matter physics. It was then realized that hydrogen-rich hydrides could also become superconductors with high critical temperatures (T_c) at substantially lower pressures than that of pure hydrogen. H_2S is converted under ultrahigh pressure (> 110 Gpa) to a metallic phase that becomes superconducting with a record T_c of ~ 200 K. It has been proposed that the superconducting phase is body-centered cubic H_3S (Im3m) resulting from a decomposition reaction $3H_2S \rightarrow 2H_3S + S$. By Appling DFT as implemented by the computer program QUANTUM ESPRESSO and by using pseudo potential approximation for electronic structure calculation for determination of density of states, Fermi energy, total energy, and electronic structure can be determine.

Dynamic response of single-crystal iron from shock compression to spall fracture using molecular dynamics simulations

N. Amadou[1] and T. De Rességuier[2]

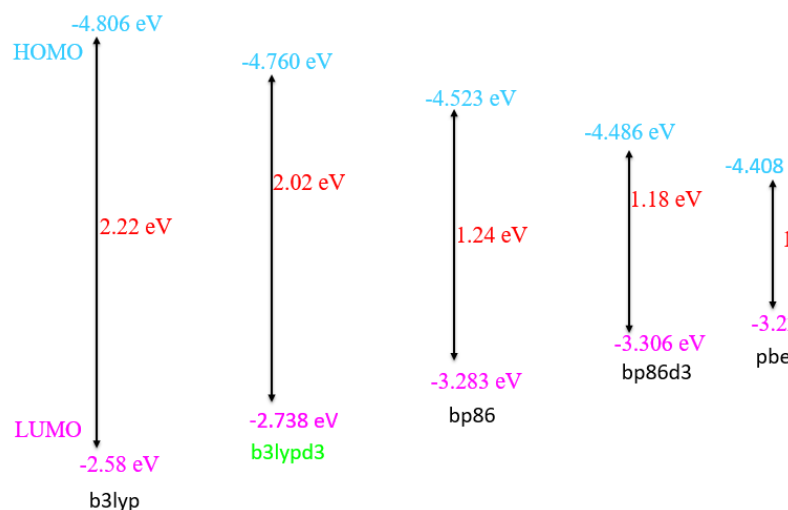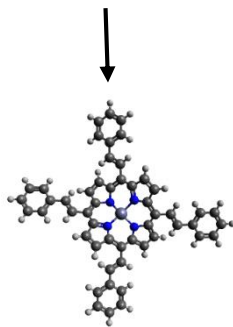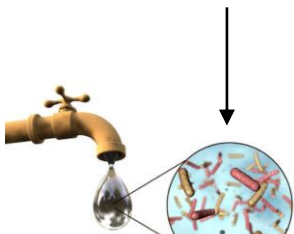[1]*Université Abdou Moumouni de Niamey, Dpt. de Physique, BP 10662 Niamey, Niger*
[2]*Institut Pprime, CNRS, ENSMA, Université Poitiers, F-86961, Futuroscope, France*

Detailed understanding of the response of solid materials to dynamic compression under extreme conditions is essential for materials science and a variety of applications[1, 2]. One typical example is iron. Indeed, being at the center of several technological applications, iron is also the main component of the core of terrestrial-like planets so that knowledge of its phase diagram is fundamental for predicting the internal structure and dynamics of such planets. Despite extensive research work, both experimental and numerical[3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14], the details of polymorphic transformations occurring in shock-loaded iron, their coupling with the high strain rate elastic-plastic behavior under both compression and release, and their influence on spall damage upon dynamic tension are not fully elucidated yet. Here, we present molecular dynamics simulations of the dynamic response of single crystal iron from shock compression to spall fracture. Behind the shock front, accompanied by twin-mediated plasticity and bcc to hcp phase transformation, as already reported extensively in the literature, the unloading wave is found to evolve into a rarefaction shock during its propagation and a pressure hysteresis between the direct and reverse phase transformations is observed. When this incident release wave interacts with the rarefaction wave reflected from the sample free surface a tensile pulse is generated within the crystal, which is found to drive a bcc to fcc phase transition whose mechanism is consistent with a Bain transformation path[15]. Depending on the tensile wave magnitude, the spall fracture process is observed to occur through voids nucleation and growth either at favorable sites (twin boundaries, bcc-fcc grain boundaries) or within the fcc phase. All these results are consistent with experimental observations including very recent ones under subnanosecond laser shock compression[16], and our simulations provide new insights into the governing mechanisms at the atomic scale and their kinetics

[1] J. R. Asay, Int. J. Impact Engng, **20**, 27 (1997).

[2] B. A. Remington, R. E. Rudd, and Justin S. Wark, Phys. Plasmas **22**, 090501 (2015).

[3] D. Bancroft, E. L. Peterson, and S. Minshall, J. Appl. Phys. **27**, 291 (1956).

[4] L. M. Barker, R. E. Hollenbach, J. Appl. Phys. **45**, 4872 (1974).

[5] J. C. Boettger and D. C. Wallace, Phys. Rev. B **55**, 2840 (1997)

[6] F. M. Wang and R. Ingalls Phys. Rev. B **57**, 5647 (1998).

[7] K. Kadau, T. C. Germann, P. S. Lomdahl, and B. L. Holian, Phys. Rev. B **72**, 064120 (2005).

[8] A. Lew, K. Caspersen, E. A. Carter and M. Ortiz, J. Mech. Phys. Solids **54**, 1276 (2006).

[9] E. B. Zaretsky, J. Appl. Phys. **106**, 023510 (2009).

[10] B. Dupré, B. Amadon, Y.-P. Pellegrini and C. Denoual, Phys. Rev. B **87**, 024103 (2013).

[11] N. Gunkelmann, E. M. Bringa, D. R. Tramontina et al., Phys. Rev. B, **89**, 140102, (2014).

[12] N. A. Zarkevich and D. D. Johnson, Phys. Rev. B., **91**, 174104 (2015).

[13] N. Amadou, T. de Resseguier, A. Dragon, and E. Brambrink, Phys. Rev. B, **98**, 024104, (2018).

[14] N. Amadou, T. De Resseguier, A. Dragon and E. Brambrink, Comput. Mater. Sci., **172**, 109318, (2020).

[15] L. H. Zhang, M. J. Cheng, X. H. Shi, J. W. Shuai, and Z. Z. Zhu, RSC Adv., **11**, 3043, (2021).

[16] H. Hwang, E. Galtier, H. Cynn et al., Science Advances, **6**, eaaz5132, (2020).

Photodynamic Antimicrobial Chemotherapy (PACT) for Water Treatment:

Synthesized Photosensitizer (PS)

-4.806 eV
HOMO

-4.760 eV

-4.523 eV

-4.486 eV

-4.408

2.22 eV

2.02 eV

1.24 eV

1.18 eV

-3.306 eV
bp86d3

-3.2
pbe

-3.283 eV
bp86

LUMO

-2.738 eV
b3lypd3

-2.58 eV
b3lyp

- The evolution of water contaminants remains a challenge to convent
- The increase in antimicrobial resistance has become a global pandem
- PACT is an alternative for antimicrobial resistance. It involves desig
  that absorb light with longer wavelength and good singlet oxygen yie

Structural, Magnetic, and Thermoelectric Properties of GdRuSi Half-Heusler Compound: A Density Functional Theory (DFT) Study.

M. Baloi[1, 2, 3*] M. Molepo[1], D. Wamwangi[1, 2, 3*]

[1] School of Physics, University of the Witwatersrand, Private Bag X3, WITS, Johannesburg, 2050, South Africa

[2] DSI-NRF Centre of Excellence in Strong Materials (CoE-SM), Physics Building, 1 Jan Smuts Avenue, Braamfontein, Johannes, South Africa

[3] Materials Physics Research Institute (MPRI), School of Physics, University of the Witwatersrand, Private Bag X3, WITS, Johannesburg, 2050, South Africa

Rare-earth based RTX (R = rare-earth element, T = transition metal, X = p-block element) half-Heusler compounds have attracted a lot of research interest due to their unique combination of physical properties desirable for application in thermoelectric, spintronic, spin caloritronic, and topological superconductivity devices [1] – [3]. This study reports on the structural, electronic, magnetic, and thermoelectric properties of GdRuSi half-Heusler compound calculated using the density functional theory (DFT) framework. The exchange correlation functional used within the generalized gradient approximation (GGA) approach is one by Perdew-Burke-Ernzerhof (PBE) as well as the revised version one for solids, that is, PBEsol. The local spin density approximation (LSDA) was adopted to investigate the collinear magnetic properties of the compound for all PBE approaches. The lattice parameters obtained within the GGA-PBEsol approach of $a = 4.1655$ Å and $c = 6.5840$ Å, for GdRuSi with a tetragonal structure, are in close agreement with experimental data ($a = 4.173$ Å and $c = 6.586$ Å) compared to those obtained with the GGA-PBE approach. We found that the magnetic moment of GdRuSi of $7.31 \, \mu_B$ for all approaches, differs slightly to the effective magnetic moment of $7.94 \, \mu_B$ for a free Gd ion. But overall, the *4f*-states of Gd contribute very significantly to the total magnetization of GdRuSi opposed to the *4d*-states of Ru and the *3p*-states of Si, as supported by the spin-polarized partial density of state (PDOS) results. The electronic band-structure and the total DOS confirms that GdRuSi is metallic in nature owing to its bandgap of $0 \, eV$ for both minority- and majority-spin channels. The thermoelectric properties will also be investigated and compared to those of rare-earth free half-Heusler counterparts XYZ (X, Y = transition elements, Z = p-block element) [4].

[1] S. Gupta and K.G. Suresh, *J. Alloys. Compd.* **168**, 562 – 606 (2015)

[2] F. Casper *et al., Semicond. Sci. Technol.* **27**, 063001 (2012)

[3] J. Ma *et al., Phys. Rev. B.* **95**, 024411 (2017)

[4] A. Hong *et al., Sci Rep* **6**, 22778 (2016)

DFT study on Pb substitution in all ignorganic-perovskites

S.Boukachabia [1] , F.Z. Bentayeb[1]

[1]*Laboratory of Magnetism and Spectroscopy of Solids (LM2S), Badji Mokhtar University, P. O. Box 12, Annaba 23000, Algeria1*

The CsBX3 perovskites, where B represents Pb, Sn, or Ge, and X represents Cl, Br, or I, have attracted considerable attention due to their potential for use in solar cells [1, 2]. In this study, we employed ab-initio calculations to investigate the electronic and structural properties of CsBX3 perovskites and to understand the effect of varying the B and X elements on their properties. Specifically, on the band structures of these materials.

It is well-established that conventional GGA calculations cannot accurately describe the band gaps of semiconducting systems [3,4]. As such, this study employs DFT with HSE06 to evaluate the energy gap of the materials. The results of the band gap are then discussed in relation to the electronegativity of B and X elements.

The study compares the energy gap values computed using GGA and HSE06 with other theoretical and experimental results. The findings reveal that all the studied alloys are semiconductors with a direct gap, and the electronic band gap is dependent on the cation B and the halogen X.

Furthermore, the study investigates the optical properties of CsBCl3, finding that Ge-based perovskites have promising potential for use in optoelectronic devices. Overall, this study provides valuable insights into the electronic and structural properties of CsBX3 solar perovskite photovoltaic materials, highlighting their potential as semiconductors and for use in solar cell devices.

[1] S. Idrissi, S. Ziti, H. Labrim, L. Bahmad, Materials Science in Semiconductor Processing, 105484, (2021).

[2] L.Xiaotong, W.Jinbo, W.Shenghao, Q.Yabing, Progress of All-inorganic Cesium Lead-free Perovskite Solar Cells, Cl 190207 (2019).

[3] C Han, L.Minghao, W.Bin, M.Sen, S.Jing, Journal of Alloys and Compounds Solar Cells, 1584442 (2021).

[4] L. Weston, H. Tailor, K. Krishnaswamy, L. Bjaalie, C.G. Van de Walle, Accurate and efficient band-offset calculations from density functional theory, Computational Materials Science, (2018)

Perovskites materials thermoelectric properties prediction with Machine Learning

Don-tsa Delchere [1] **, Messanh A. Mohou** [1] **, Katawoura Beltako** [1]

[1]*University of Lome, Faculty of Sciences, Department of physics, Laboratory of Physics of Semiconductor Materials and Components (LPMCS)*

The high computational demand of the Density functional Theory based (DFT) method for screening new properties or materials remains a strong limitation to the development of clean and renewable energy technology essential to transition to a carbon-neutral environment in the coming decades. In this situation, Machine Learning comes into play with its innate capacity to handle huge amounts of data and high-dimensional statistical analysis. In this study, machine learning methods (Random Forest and Artificial Neural Network) are used to predict the thermoelectric properties of perovskite materials. The aim is to analyze and understand the behavior of these materials in order to optimize their properties for prediction of higher performing thermoelectric materials. Random Forest Algorithm (R^2=0.902) shows higher accuracy compared to Artificial Neural Networks (R^2=0.817) for property prediction. This study pave the way for the use of Random Forest algorithm in predicting good thermoelectric materials based on their chemical composition.

Key words: Perovskites, Thermoelectric, Prediction, Machine Learning

Dirac plasmon in novel topological semimetals: insights from ab-initio calculations

Wala Elsayed (1), Ridwan Agbaoye (2), Maram Ali Ahmed (3),
Timothy Ashani (4), Bruno Dandogbessi (5), Mohamed
El Kinawy (6), Fatema Mohamed (7), Menberu Woldemariam (8), Andrea Marini (9),
Matteo Gatti (10).

*(1) ICTP-EAIFR, Rwanda, (2) Federal College of Dental
Technology and Therapy, Nigeria, (3) National Ribat University,
Sudan, (4) Federal University of Agriculture, Nigeria, (5) IMSP,
Benin, (6) Ain Shams University, Egypt, (7) University of Khartoum, Sudan
(8) Jimma University, Ethiopia, (9) ISM-CNR, Italy, (10) LSI CNRS
Ecole Polytechnique, France*

Three-dimensional (3D) topological Dirac semimetals have received researchers' attention recently. Along with possessing 3D Dirac fermions in the bulk, they represent a unique state of quantum matter that can be seen as 3D graphene. In recent years, ternary and binary alkali pnictides compounds, $Li_{3-x}Na_xM$ (x = 3, 2, 1, 0; M = N, Sb, Bi), were identified as new topological Dirac materials [1,2]. They show different types of band dispersions around the symmetry-protected 3D Dirac points. Therefore they offer an ideal platform to investigate Dirac plasmons that hold great potential for plasmonic applications [3]. So far, the predictions of Dirac plasmon properties have been based mostly on simplified models representing the band dispersion only around the Dirac points [4]. In our work, based on ab initio time-dependent density functional theory simulations, we instead take into account both the contributions from the whole band structure and the effects of the electron-electron interaction. We obtain an accurate and realistic description of the plasmon dispersion in the alkali pnictides, which allows us to draw a detailed picture of plasmon properties in different types of Dirac materials.

References

[1] Z. K. Liu, et al. Science **343**, 864 (2014).
[2] L. Jin, et al. Physical Chemistry Chemical Physics **22**, *5847* (2020).
[3] A. Politano et al. Phys Rev Lett. **121**, 086804 (2018). See also Physics **11**, s99.
[4] K. Sadhukhan, A. Politano, and A. Agarwal. Phys. Rev. Lett. **124**, 046803 (2020) -

FIRST PRINCIPLES STUDY OF DEFECTS ADSORBED ON BOROPHENE CRYSTAL STRUCTURE FOR HIGH PERFORMANCE LITHIUM AND SODIUM BATTERIES.

Chewe Fwalo [(a)*, (b)] and Refilwe Edwin Mapasha[(b)]

[(a)] Physics Department, Copperbelt University, Kitwe 10101, Zambia

[(b)] Physics Department, University of Pretoria, Pretoria 002, South Africa

The unique properties of the 2D materials such as good electrochemical potential, large surface area etc, have made 2D materials such as borophene to be explored further in the search for high energy and power densities of lithium and sodium batteries. In our study, main aim is to study effect of defects adsorbed on borophene crystals as anode material for high performance lithium and sodium batteries,through first principles study and density functional theory (DFT) calculations .The objectives are to investigate the electrical and structural properties of defected borophene allotropes (Striped,Beta-12 and Chi-3). Furthermore, anode material properties such as diffusion energy barrier, open circuit potential, specific capacity storage, adsorption energy ect. will be monitored. Ascertaining dynamical stability of defected borophene structures, phonons will be calculated using Phonopy code and analyze the phonon dispersions. Other stability properties to be considered are thermodynamical and mechanical of the defected borophene allotropes. Our preliminary results of the lattice parameters of the aforementioned borophene structures agrees well with the other experimental and theoretical data previously found; Striped (a= 1.624 ang, b=2.866 ang), Beta-12 (a=3.1 ang, b= 5.207 ang) and Chi-3 (a= 2.928 ang, b= 8.512ang) after geometry optmisation and before defects adsorption. All in all, once the investigated properties match with properties of the commercialized graphite and other 2D materials reported,then the proposed structures will be promising anode materials for high performing future energy storage systems or Lithium and Sodium batteries.

Keywords: density functional theory; defects; defected borophene allotropes; lithium and sodium batteries.

References

[1] W. Kohn and L. J. Sham, Phys. Rev. 140, A1133 (1965).

[2] P. Hohenberg and W. Kohn, Phys. Rev. 136, B864 (1964).

[3] J.P. Perdew, K. Burke, M. Ernzerhof, Generalized gradient approximation made simple, Phys. Rev. Lett. 77 , 3865–3869 (1996).

[4] X. Gonze, C.Y. Lee, Dynamical matrices, Born effective charges, dielectric permittivity tensors, and interatomic force constants from density-functional perturbation theory, Phys. Rev. B: Condens. Matter Mater. Phys. 55,10355–10368 (1997).

First-Principles Insights into Electric-Field Induced Phase Transition in Magnetic Tunnel Junctions

<u>Musa A. M. Hussien</u>[1,2] and **Aniekan M. Ukpong**[2]

[1]*Department of Physics, Faculty of Science and Technology, Omdurman Islamic University, Omdurman P.O. Box 382, Sudan*
[2]*Theoretical and Computational Condensed Matter and Materials Physics Group (TCCMMP), School of Chemistry and Physics, University of KwaZulu-Natal, Pietermaritzburg 3201, South Africa*

In this study, we investigate the emergent collective properties of feromagnetic metal-insulator-metal heterostructure materials in perpendicular magnetic tunnel junctions. Using an effective field theory that combines density functional theory and spin-polarized conductance calculations, we explore the proximity effect induced magnetoelectric couplings in spin transport with a monolayer tunnel barrier material. Our findings reveal a discontinuous change in the spin density of states from half-metallic to metallic with the application of an electric field, resulting in an electric-field induced quantum phase transition. This study highlights the importance of the choice of tunnel barrier layer material in determining magnetoelectric couplings during spin tunneling under external field bias.

[1] M. Hussien, A. Ukpong, Nanomaterials, **12**, 1836 (2022).

Quantum Computing for Electronic Structure Calculations

Nouhaila INNAN [1] , Mohamed BENNAI [1,2]

[1] *Quantum Physics and Magnetism Team, LPMC, Faculty of Science Ben M'sick,*
Casablanca Hassan II University, Morocco.
[2] *Lab of High Energy Physics, Modeling and Simulations, Faculty of Science, University*
Mohammed V-Agdal, Rabat, Morocco

Electronic structure calculations are a critical tool for understanding the behavior of materials at the quantum level. However, traditional electronic structure methods can be computationally expensive, limiting their applicability to large or complex systems. In this poster, we present a novel quantum algorithm for electronic structure calculations and demonstrate its performance using state-of-the-art quantum computing hardware. Our quantum algorithm is based on the variational quantum eigensolver (VQE) algorithm, which we modify to perform electronic structure calculations by mapping the quantum system to a set of qubits and using a quantum circuit to prepare the ground state wavefunction. We demonstrate the performance of our algorithm using a variety of benchmark systems. We show it can achieve comparable accuracy with significantly fewer computational resources than traditional electronic structure methods. Our work offers a potential solution to the challenge of computationally expensive electronic structure methods. It demonstrates the power of quantum computing for accelerating the development of new materials and technologies.

Density-functional study of the thermodynamic properties and the pressure-temperature phase diagram of Mg_2SiO_4

Omamuyovwi Rita Jolayemi[1] and Davide Ceresoli[2]

[1]*Department of Physics, College of Science and Technology, Covenant University, Ota, Ogun State, Nigeria*

[2]*Consiglio Nazionale delle Ricerche - Istituto di Scienze e Tecnologie Chimiche "G. Natta" (CNR-SCITEC), via Golgi 19, 20133, Milano, Italy*

First-principles ab initio calculations [1] were used to explore the structural and vibrational behaviour of Mg_2SiO_4 under compression. We show that at 10GPa and 12.2GPa, Mg_2SiO_4 experiences a pressure-induced phase shift from Pnma $\rightarrow$ Imma $\rightarrow$ F3dm structure, respectively. The dynamic stablities of the structures of Mg_2SiO_4, $MgSiO_3$ and MgO were examined by phonon spectrum calculated through finite displacement method [2]. We found that the Pervoskite structure, $MgSiO_3$ (space group Pm3m) as well as the Wadsleyite crystal (space group Imma) are thermodynamically unstable due to frequencies less than zero. As a result, we used the free energy-based renormalisation scheme [3], which allows DFT to calculate vibrational free energy even for materials having negative curvature of the potential energy surface in relation to atomic displacement. Furthermore, Kieffer's model depicted the vibrational density of states and thermodynamic features of pure substances in pressure-temperature space.

[1] P. Giannozzi, S. Baroni, N. Bonini, M. Calandra, R. Car, C. Cavazzoni, D. Ceresoli, G. L. Chiarotti, M. Cococcioni, I. Dabo, A. Dal Corso, S. Fabris, G. Fratesi, S. de Gironcoli, R. Gebauer, U. Gerstmann, C. Gougoussis, A. Kokalj, M. Lazzeri, L. Martin-Samos, N. Marzari, F. Mauri, R. Mazzarello, S. Paolini, A. Pasquarello, L. Paulatto, C. Sbraccia, S. Scandolo, G. Sclauzero, A. P. Seitsonen, A. Smogunov, P. Umari, R. M. Wentzcovitch, QUANTUM ESPRESSO: a modular and open-source software project for quantum simulations of materials. J. Phys. Condes. Matter. **21**, 395502 (2009).

[2] A. Togo and I. Tanaka. First principles phonon calculations in materials science. Scr. Mater. **108**, 1–5 (2015).

[3] D. J. Adams and D. Passerone. Insight into structural phase transitions from the decoupled anharmonic mode approximation. Journal of Physics: Condensed Matter. **28**, 305401 (2016).

Transition Metal Complexes for alternative drug synthesis as antibacterial and Antioxidant Activities: A Combined Experimental, DFT, and Molecular Docking Studies

Tadewos Damena[1]*, Mamaru Bitew[2], Digafie Zeleke[3], Tegene Desalegn[2] and Taye B. Demissie[4]

[1]Department of Chemistry, Wachemo University, P.O. Box 667, Hossana, Ethiopia.

[2] Department of Applied Chemistry, Adama Science and Technology University, P.O. Box 1888, Adama, Ethiopia.[3]Department of Chemistry, Salale University, P.O. Box 245, Fitche, Ethiopia

[4]Department of Chemistry, University of Botswana, Notwane Rd, P/bag UB 00704 Gaborone, Botswana

***Corresp. Author**: Dr. Tadewos Damena,.tad.dam.keb2010@gmail.com: phone: +251913334291*

Abstract

Heterocyclic quinoline like ligand having imine is important biologically active organic molecules that have attracted attention of bioinorganic, pharmaceutical and medicinal chemists due to their wide range of pharmacological properties and familiar coordination behaviour. In this work, series of four new metal complexes: Zn(II), Cu(II), Co(II) and Ni(II) were prepared from 2-chloroquinoline-3-carbaldehyde. The compounds were characterized with physicochemical and spectroscopic methods. The analyses were supported with DFT and TD-DFT calculations and in very good agreement with experimental results [1–4]. *In vitro* antibacterial activity analysis of the complexes were studied with disc diffusion methods, and all the complexes exhibited very good activities with *Pseudomonas aeruginosa* (18.90 ± 2.06 - 20.90 ± 2.05 mm diameter at concentration of 200 μg/mL, respectively), among these Cu(II) complex showed higher percent activity index against both *Escherichia coli,* and *Pseudomonas aeruginosa*. The complexes were also evaluated for their antioxidant properties and showed higher antioxidant activities. Among these: Cu(II) and Zn(II) complexes exhibited better antioxidant activities with IC_{50} values of 8.62 and 4.70 µg/mL, respectively[2,3]. Overall, the newly synthesized Zn(II), Cu(II) and Co(II) complexes have biological activities, with the Cu(II) complexes having much better activity than other complexes and these result were found to be in good agreement with binding mode against *E. coli* DNA gyrase B[1–4]. The higher antibacterial activity of Cu(II) complex against Gram-negative bacteria makes the complex potential alternative drug for treating diseases caused by Gram-negative bacteria after passing cytotoxicity testing. In other ways the compounds that can scavenge DPPH radicals might exhibit anticancer, antiaging, anti-inflammatory activities. Hence our complexes have pronounced DPPH radical scavenging activities, they may have the anticancer and antidiabetic related activities and the door is open for any interested researchers.

References

1   A. Z. El-Sonbati, M. A. Diab, S. M. Morgan, M. I. Abou-Dobara and A. A. El-Ghettany, *J. Mol. Struct.*, 2020, **1200**, 127065.

2   A. Z. El-Sonbati, N. F. Omar, M. I. Abou-Dobara, M. A. Diab, M. A. El-Mogazy, S. M. Morgan, M. A. Hussien and A. A. El-Ghettany, *J. Mol. Struct.*, 2021, **1239**, 130481.

3   I. A. I. Ali, S. S. A. El-Sakka, M. H. A. Soliman and O. E. A. Mohamed, *J. Mol. Struct.*, 2019, **1196**, 8–32.

4   M. Ismael, A. M. M. Abdel-Mawgoud, M. K. Rabia and A. Abdou, *Inorg. Chim. Acta*, 2020, **505**, 1–11.

The effect of pressure on electron-phonon interaction in metallic systems: case of MgB$_2$

Willy Bellard KIRA

Doctoral School of University of Burundi, Bujumbura, Burundi

The effect of pressure on electron-phonon interaction was investigated in metallic system MgB$_2$. The electronic and phonon properties were derived from first principles calculations within density functional theory (DFT) and density functional perturbation theory (DFPT), as implemented in Quantum Espresso package. Superconducting properties (electron-phonon coupling, spectral function…) were studied using Migdal-Eliashberg formalism and computed with EPW code incorporated in Quantum Espresso. The results show that applying pressure on hexagonal MgB2 decrease electron-phonon interaction. This monotonic decrease comes from the E2g modes of Boron atoms around Γ point. Electron-phonon coupling found to be decreasing also from 0.667 at o kbar to 0.229 at 953 kbar. Our study will allow the comparative study by applying negative pressure to the same system, to evaluate the increasing of electron-phonon interaction, which would be applied to various strain-engineering problems in functional materials.

[1] P. Giannozzi et al, J. Phys. : Condens. Matter. **21**, 395502 (2009)
[2] F. Giustino, Rev. Mod. Phys. **89**, 015003 (2017).
[3] E.R. Margine, F. Giustino, Phys. Rev. B **87**, 024505 (2013).
[4] Z.D. Gerbi, P. Singh, AIP Advances **9**, 095038 (2019).
[5] E. Johanson et al, J. Appl. Phys. **131**, 063902 (2022).

Temperature-dependent mechanical properties of graphynes and applications: Machine Learning vs classical potential

<u>Jacques Kotoko</u>[1], Komi Sodoga[1], Yusuf Shaidu[2], Seriani Nicola[3], Katawoura Beltako[1]

[1] Université de Lomé, Faculté des Sciences, Département de physique, Laboratoire de Physique des Matériaux et Composants à Semi-Conducteurs (LPMCS)

[2] The Abdus Salam ICTP, I-34151, Trieste, Italy

[3] University of California, Berkeley

In this research work, we study the temperature-dependent mechanical properties of differents graphynes (6-6-6-, 6-6-12-, 14-14-14- and 14-14-18-graphyne), under tension of uniaxial, biaxial and shear tensile strength using different classical potentials (REBO [1], AIREBO [2], AIREBO-M [3]) against a machine learning based potentiel (PANNA [4]). Elastic properties such as Young's, shear and bulk moduli as well as Poisson's ratios are investigated using molecular dynamics simulations as implemented in LAMMPS [5]. The results show that the different potentials predicted at 15% error the experimental values. The results also indicate that PANNA performs less accurately compared to classical potentials. In conclusion, the results of this study highlight the importance of Machines learning based potentials for fast and accurate mechanical properties prediction.

[1]   Brenner, Shenderova, Harrison, Stuart, Ni, Sinnott, J Physics: Condensed Matter, 14, 783-802 (2002)

[2]   Stuart, Tutein, Harrison, J Chem Phys, 112, 6472-6486 (2000)

[3]   O'Connor et al., J. Chem. Phys. 142, 024903 (2015).

[4]   Lot R., Pellegrini F., Shaidu Y., & Küçükbenli E. (2020). Panna: Properties from artificial neural network architectures. *Computer Physics Communications, 256*, 107402

[5]   S. Plimpton, Fast Parallel Algorithms for Short-Range Molecular Dynamics, J. Comp. Phys. 117 1-9 (1995). URL: http://lammps.sandia.gov

Ab initio calculations on optoelectronic properties of lead-free double halide (elpasolite) perovskite Cs$_2$AgBiI$_6$

<u>Patience M.</u> [1] , Victor O. [1] , and Celine A.[1]

Department of Physics, Masinde Muliro University of Science and Technology [1]

A recent surge in studies towards alternative lead-free perovskite materials has been driven by concerns about toxicity and instability of lead-halide perovskites. To date the search for a non-toxic, stable halide perovskite with great photo-conversion efficiency [1,2;3] is a major challenge.

In this work we study lead-free double halide Cs$_2$AgBiI$_6$ material with a visible bandgap which is an alternative to current perovskite standout CH$_3$NH$_3$PbI$_3$ [4].We are to investigate the structural and opto-electronic properties and stability using Goldschmidt[5] tolerance factor and Bethe-Salpeter[6] equation in Yambo code of cubic material, a double perovskite material that has recently shown good opto-electronic trends which are of interest in this study.

A double perovskite is a material that can host two different transition metal cations at the B-sites of its perovskite structure[4] . First principle calculations are to be employed through Quantum Espresso and Yambo codes in the Density Functional Theory perspective. Results obtained are to be compared against experimental and theoretical data and that from other code combination.

REFERENCES

[1] A.J Pearson, G.E Eperon., et al., Advanced Energy Materials, 2016;

[2] M. Alsari, A.J Pearson et al., *Scientific reports*, *8*(1), 5977, 2018;

[3] M. Alsari, O. Bikonda et al., *Energy & Env Science, 10.1039.C7EE03013D* 2018

[4] Mark T, Anderson et al., Progress in Solid State Chemistry, 1993

[5] Goldschmidt 1926

[6] S. Albrecht , G. Onida et al., Phys. Rev. B **55**, 10278, 1997

STRUCTURAL AND ELECTRONIC PROPERTI
DISULFIDE: A DENSITY FUNCTION

G.M. Mumbi
Department of Mathematics, Physics and C
K.K. Korir
Head of Department of Mathematics, Physics ar
N.W. Makau
Department of Physics, Univers

Recent research shows that the structural and electronic properties of bulk MoS
electronic properties of bulk Molybdenum Disulfide have been investigated using th
Disulfide is a dark, shinny solid which occurs naturally as the mineral 'Molybde
structure consisting of S-Mo-S. The bonding between these two compounds is a cov
forces. It has two such layers where Mo is sandwiched between two sulfur atoms an
electronic devices such as the FETs [3]. This work used the DFT framework, usi
iterations were performed on the bulk MoS2 and the values were obtained at a con
sampling for the brillouin basis was set at 8x8x4 and the kinetic energy cut-off was se
(lattice parameter, a) and 4.30 (c/a ratio) [2]. The optimized structure was found to be
values had a small deviation from the experimental values (0.3%). The results of bon
deviation) whereby a shorter bond length shows the material is strong. The bond ang
obtained had an indirect band gap of 1.06eV which coincides at the top of the valen
the midpoint of the axis of symmetry of Gamma and K(G-K). Bulk MoS2 is an indir
Bond angles help in determining the shape of the material and give an insight about t
Bond length and bond angles for this study were determined using the xcyrsden s
experimental values where both values vary with a small deviation. The structure obta

REFERENCES

1. Ahmad, Sohail & Mukherjee, Sugata. (2014). A Comparative Study of Electronic Pr
   Technique: Application of Mechanical Strain on MoS2 Monolayer. Graphene. 03. 5

2. Perdew J., Burke K., and Ernzerhof M. 1996.

3. Manzeli, S., Ovchinnikov, D., Pasquier, D. et al. 2D transition metal dichalcogenide
   https://doi.org/10.1038/natrevmats.2017.33

4. Kohn W. and Sham L. J., "Self-consistent equations including exchange and correla
   (Nov 1965).

Enzyme encapsulation for carbon dioxide capture and conversion in MOFs

Gadzikano Munyuki [1] and Gift Mehlana [2]

[1](Presenting author underlined) Chinhoyi University of Technology, Chinhoyi, Zimbabwe
[2] Midlands State University, Gweru, Zimbabwe

The methanol economy is vital to addressing growing global needs for improved energy storage whilst reducing carbon emissions [1]. The production of methanol from CO_2 under heterogeneous conditions has been done using $Cu/ZnO/Al_2O_3$ composites[2]. These composites require harsh conditions making catalyst structure difficult to control. Recently, however, advances in our understanding of enzymatic processes have suggested applications in the energy sector. Hence, the CO_2-methanol cycle comprises a cascade reaction involving formate dehydrogenase (FDH), formaldehyde dehydrogenase (FalDH) and alcohol dehydrogenase (ADH) [3]. Glutamate dehydrogenase then regenerates the system by reducing NAD^+ to nicotinamide adenine dinucleotide. This suggests a new approach to CO_2 recycling into methanol, which can be used to replace oil in the chemical industry, or alternatively, CO_2 can be captured and stored in (hopefully) other long-lived products.

The instability, short shelf-life, and difficulty of recycling enzymes can inhibit their application. These problems can be overcome by immobilization on solid supports[4], offering a high enzyme-to-substrate ratio, efficient digestion, and easy handling.

Metal-organic frameworks (MOFs) self-assemble from metal nodes and organic linkers. Pore sizes up to ~6 nm can result, with high apparent surface areas and guest storage capacities. This makes them attractive for adsorbing guests (enzymes) on their internal surfaces. They offer stability, recyclability, and size/conformation control over encapsulated guests. MOFs have been developed as enzyme supports to give enzyme@MOF composites[4]. These offer tunable porosity to prevent leaching, uniform enzyme loading throughout the host, and control over the enzyme microenvironment.

Most of the current computational studies of biomolecule@MOF systems are mainly limited to the model MOF IRMOF and small molecules such as peptides and single amino acids.

This work sought to detail the atomic level mechanism of encapsulation and covalent linkages of formate dehydrogenase in a water soluble MOF, UiO-66. GROMACS, LAMMPS and Gaussian software packages were used.

References
1. J. Graciani, et al. Science 2014, 345, 546-550.
2. X. Zhang, et al. Fuel 2010, 89, 1348-1352
3. J. Shi, et al. Chem. Soc. Rev. 2015, 44, 8877-8903.
4. J. Mehta, et al. Coord. Chem. Rev. 2016, 322, 30-40.

Investigation of Magnetic properties of FeMnPIn using GGA functionals

Abstract

Magnetic properties of stable iron-based compounds (FeMnP1-xAx (A = Si, In) were investigated by use of Quantum Espresso (QE) within the Density Functional Theory (DFT) formalism as a viable magnetic refrigerant. In this research work, DFT technique was the first principle theoretical approach that was employed along with the planewave pseudopotentials (ultrasoft), and the projected augmented wave (PAW) within the generalized gradient approximation (GGA) to describe the electronic structure and investigation of magnetic properties. Magnetic stability is described as the repeated magnetic performance of a material under specific conditions over the life of a magnet. In, was chosen to replace silicon since they would easily mimic the bond, their availability and nontoxic nature. The results showed In is suitable replacement of Si and its magnetic phases showed stability.

Influence of the pH of Anthocyanins on the Efficiency of Dye Sensitized Solar Cells

Alex Okello [a], Brian Owino Owuor [b], Jane Namukobe [c], Denis Okello [a], Julius Mwabora [b]
[a]Department of Physics, Makerere University, P.O. Box 7062 Kampala, Uganda
[b]Department of Physics, University of Nairobi, P.O. Box 30197-00100, Nairobi, Kenya
[c]Department of Chemistry, Makerere University, P.O. Box 7062, Kampala, Uganda
Corresponding Author: Alex Okello
Email Address: alex.okello@mak.ac.ug

Abstract

The influence of the pH of anthocyanins on photovoltaic performance in dye-sensitized solar cells has been investigated. Anthocyanins were extracted from crushed leaf stocks of *Manihot esculenta* Crantz (Cassava plant) using methanol acidified with 0.5% trifluoracetic acid. The filtrate was concentrated using a rotary evaporator and partitioned against ethyl acetate. The anode was prepared by screen printing TiO_2 paste on a previously cleaned fluorine-doped tin oxide (FTO) glass substrate. The cathode was made by applying plastisol on a previously cleaned FTO glass substrate using an artistic brush and later annealed at 450 °C for 20 minutes to activate platinum. The performance of the solar cells was measured using a solar simulator fitted with an AM1.5 air filter. Electron transport was studied using electrochemical impedance spectroscopy (EIS). It was observed that the short circuit current and efficiency dropped from pH 2 to pH 6 and peaked at pH 8, with values of 0.399 mA and 0.390%, respectively. It then drops further as the basicity increases. The open circuit voltage was observed to increase consistently from pH 2 to pH 12. EIS results showed that the electron density in the conduction band of TiO_2 increases from pH 2 to pH 10 and drops from pH 10 to pH 12. It was concluded that, while a large number of electrons ($\sim 10^{16} m^{-3}$) are injected into the conduction band of TiO_2, the majority do not contribute to the current but instead recombine with other electron acceptor species in the solar cell. However, the injected electrons cause an upwards shift in the quasi-Fermi level of electrons in the conduction band of TiO_2. This explains the large variation in the open circuit voltage compared to the short circuit current.

Key words:

Electron density, TiO_2, electron lifetime, screen printing, dye detachment, pH

Electronic and optical properties of antiperovskites: The GW/BSE approach

E. Oyeniyi [1]

[1]Department of Physics, University of Ibadan, Nigeria

Antiperovskites (APs) have several potential applications. Methods based on Density Functional Theory (DFT) have been mostly utilized to study their properties. In this work, the GW and solution to the Bethe Salpeter Equation (BSE) were employed to study the electronic and optical properties of Mg_3XN (X= P, As, Sb, Bi) APs. The Mg_3XN (X= P, As) were found to have direct band gaps, while Mg_3XN (X= Sb, Bi) have indirect gaps. The G_0W_0/eVGW band gaps for the antiperovskite are in the range the 1.29-2.33/1.47-2.61eV. The inclusion of the spin-orbit coupling (soc) reduced the G_0W_0/eVGW band gaps by 40/33% and 15/13% for Mg3SbN and Mg3BiN, respectively. The optical properties of the APs from the solution to BSE show that they could serve as good materials for solar cell applications and optoelectronic devices.

Density-Functional Theory Study of the Reactivity of Buckminsterfullerene towards Hydroxyl Radicals

Abraham Ponra[1], Anne Justine Etindele[2], Mark E. Casida[3], and Ousmanou Motapon[1]
1: Physics Department, University of Maroua, Cameroon
2: Higher Teachers Training College, University of Yaounde I, Yaounde, Cameroon
3: Département de Chimie Moléculaire (DCM), Université Grenoble Alpes (UGA), Grenoble, France
*email: abraponra@yahoo.com

Introduction

C_{60} has been called a "radical sponge" because of its remarkable ability to react with radicals, which makes it an excellent candidate as an antioxidant for combating the deleterious effects of reactive oxygen species. Previous studies have focused on characterizing the products of the reaction of C_{60} with the $^\bullet$OH radical. Here we focus on which factors govern the regioselectivity of $^\bullet$OH radical reactions upon successive addition to $C_{60}(OH)_n$. We demonstrate the complex, but still comprehensible, interplay of charge, unpaired spins, and Fukui functions, in determining where the $^\bullet$OH radical reacts.

Method and Computational Details

Kohn-Sham density-functional theory (DFT) is used for ground-state calculations

$$\left[-\frac{1}{2}\nabla^2 + V_{ex}(r) + V_H(r) + \frac{\partial E_{xc}[\rho]}{\partial \rho(r)} \right] \varphi_i(r) = \varepsilon_i \varphi_i(r)$$

The calculations have been done at B3LYP/def2-SVP level using the Programs Orca (4.2.1 version).
The main descriptors studies for descripting the successive fixation

- Fukui charges
$$f_I^- \approx q_I(N-1) - q_I(N)$$
$$f_I^+ \approx q_I(N) - q_I(N+1)$$
$$f_I^0 \approx (q_I(N-1) - q_I(N+1))/2$$
$$\Delta f_I \approx q_I(N-1) - 2q_I(N) + q_I(N+1)$$

- spin density $\rho_\uparrow - \rho_\downarrow$
- Bond Dissociation Energy (BDE)

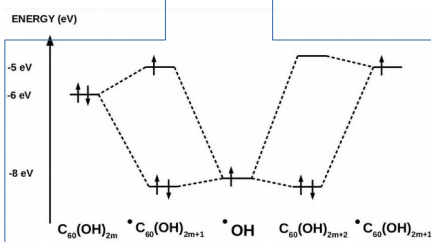$$E(A\text{-}B) - [E(A) + E(B)] = \Delta E = E_{RCF} + E_{Coul} + E_{FMO}$$
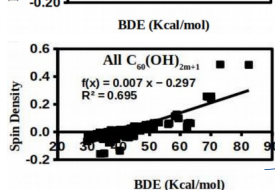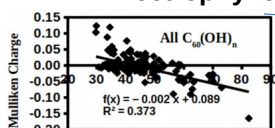
Results

With fullerenol $C_{60}(OH)_n$

$$C_{60}(OH)_{2m} + {}^\bullet OH \rightarrow {}^\bullet C_{60}(OH)_{2m+1}$$
$$^\bullet C_{60}(OH)_{2m+1} + {}^\bullet OH \rightarrow C_{60}(OH)_{2m+2}$$

$^\bullet$OH is an electrophilic radical

$^\bullet$OH are subdivided as nucleophilic and electrophilic

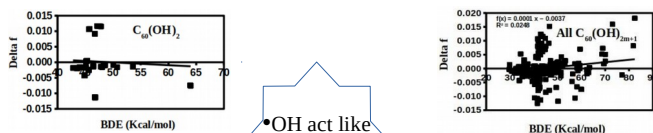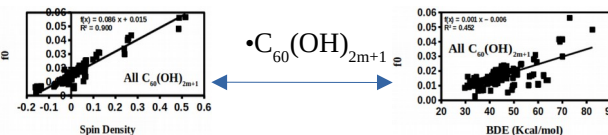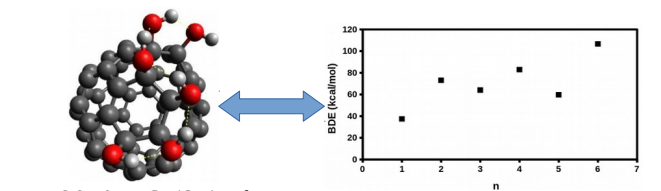Rough FMO correlation energy diagram

Electrophylic character

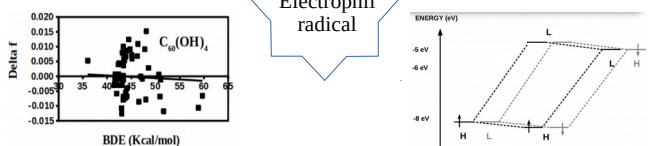All $C_{60}(OH)_n$
f(x) = − 0.002 x + 0.089
R² = 0.373

All $C_{60}(OH)_{2m+1}$
f(x) = 0.007 x − 0.297
R² = 0.695

The orbital control

Regioselectivity

$C_{60}(OH)_2$ 26   5,10

$C_{60}(OH)_4$ 2,4,7,8   10,20

$C_{60}(OH)_{2m+2}$

All $C_{60}(OH)_{2m+1}$
f(x) = 0.086 x + 0.015
R² = 0.900

All $C_{60}(OH)_{2m+1}$
f(x) = 0.001 x − 0.006
R² = 0.452

$^\bullet C_{60}(OH)_{2m+1}$

$C_{60}(OH)_2$

All $C_{60}(OH)_{2m+1}$
f(x) = 0.0001 x − 0.0037
R² = 0.0248
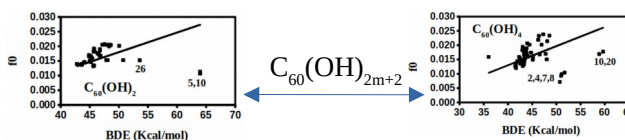
$^\bullet$OH act like Electrophil radical

$C_{60}(OH)_4$

1,5,6,9,10,11-$C_{60}(OH)_6$, the most stable isomer found in this study

BDE of $(^\bullet)C_{60}(OH)_n$ as a function of n

Conclusion & Perspectives

It is confirmed that the $^\bullet$OH radical is very electrophilic. Thus it will react with unpaired spins (spin density) of the fullerenol $^\bullet C_{60}(OH)_{2m+1}$ and there will also be a correlation with charge density. But it is the Fukui function and the dual descriptor that say most clearly that the regioselectivity is determined by the electrophilic nature of the OH radical when the hydroxyl radical ($^\bullet$OH) react whith the fullerenol $C_{60}(OH)_{2m}$.

For further information, see our preprint on the arXiv:

Stability, electronic and structural properties of aluminene
from first-principles calculations

Pape SENE [1,2] , **Allé DIOUM** [1,2] , **Sossé NDIAYE** [2] , **El Hadji Oumar GUEYE**[2],
KharounaTALLA[2] , **and Aboubaker Chédikh BEYE** [2]

[1]*Laboratory* of *Materials – Composite Systems and Applications
(MASCA),Department of Physics, Cheikh Anta Diop University (UCAD), Dakar,
Senegal*
[2]*Physical Solid and Material Sciences Group, Department of Physics, Cheikh Anta
Diop University of Dakar, 5005 Dakar, Senegal*

In this paper, we study the stability of aluminene, a two-dimensional monolayer aluminum structure. In fact, we use the density functional theory to study the stability of four differents configurations of aluminene: hexagonal (graphene), buckled (silicene), Trigonal (space group p3ml) and orthorhombic (space group pmmn). The dispersion spectrum shows that only the graphene-like aluminene and the silicene-like aluminene were stable. Their electronic structure has shown that both graphene-like and silicene-like structures have a metallic behavior. The Compression and stretching of those stable structures revealed that the graphene-type configuration is stable up to 10% compression and 29% stretching. The silicene configuration starts to become unstable at 3% (stretching) however; it remains stable up to 15% compression.

Rovibrational states calculations of the H_2O-HCN heterodimer with the Multiconfiguration Time Dependent Hartree method.

Hervé Tajouo Tela[a], Ernesto Quintas Sánchez[b], Marie-Lise Dubernet[c], Yohann Scribano[d], Richard Dawes[b], Fabien Gatti[e], Steve Ndengué[a*]

[a]*ICTP-East African Institute for Fundamental Research, University of Rwanda, Kigali, Rwanda*
[b]*Department of Chemistry, Missouri University of Science and Technology, 65409 Rolla, Missouri, United States.*
[c]*LERMA, Observatoire de Paris, PSL Research University, CNRS, Sorbonne University, UPMC Univ Paris 06, 92190 Meudon, France.*
[d]*Laboratoire Univers et Particules de Montpellier, UMR-CNRS 5299, Université de Montpellier, Place eugène Bataillon, 34095 Montpellier Cedex, France*
[e]*Institut de Sciences Moléculaires d'Orsay, UMR-CNRS 8214, Université Paris-Sud - Université Paris-Saclay, 91405 Orsay, France*

E-Mail: sndengue@eaifr.org

Abstract

Water, also called the molecule of life is the most abundant polyatomic molecule in the galaxy and the 3rd most abundant molecule in the Interstellar Medium (ISM) after CO and H_2. In the recent years, mixed H_2O – HCN heterodimer have attracted a great number of experimentalists and theorists alike with a special interest on its structure and spectroscopy but no complete quantum calculations of the rovibrational states have been done. Here we will present the rovibrational states of the H_2O – HCN in the rigid rotor approximation for $J = 0, 1, 2, 3$ total angular momentum, quantum numbers using the five-dimensional(5D) potential energy surface with the MultiConfiguration Time Dependent Hartree (MCTDH) method.

Temperature dependence on the interband transition in single modified droplet epitaxy GaAs/Al0.3Ga0.7As quantum dots

M. Triki

Laboratoire de Physique de la Matière Condensée, Faculté des Sciences de Tunis, Université de Tunis El Manar, Tunis, Tunisia

Semiconductor quantum dots (QD) are nanocrystals in which quantum size confinement effects are observed. Since their discovery, they have attracted significant attention as beneficial candidates in several applications. Nowadays, they become potentially basic elements for a wide variety of optoelectronics devices such as lasers, bio-labling, solar cells,... Coupling of QD's localized-carriers with their environment represents, however, one of the most severe obstacles for implementation of true quantum devices, mainly, if QDs are to be used in devices sensitive to dephasing and loss of coherence such as quantum information devices. Such coupling leads to decoherence that is evidenced in PL-spectra. These later show lateral sidebands with a zero phonon line width much larger than the radiative limit.

Temperature dependence on the ground interband transition in GaAs/Al0.3Ga0.7As modified droplet epitaxy (MDE) quantum dots (QDs) is investigated. Results show that, the macro-atom scheme of QDs survives only at low temperature and the coherence of the interband transition decays with temperature. In fact, coupling with acoustic phonons leads to the presence of the phonon wings and the quenching of the zero phonon line (ZPL) intensities. Despite of this phononic disturbance, we find that, GaAs/Al0.3Ga0.7As MDE QDs still remain better than other proposed candidates for application in devices needing more coherence.

First principles study of Electronic, Structural, Phonon and Thermodynamic properties of XCrSb (X= Fe, Os) half-Heusler spintronic compounds

Oghenekevwe T. Uto[1], Paul O. Adebambo[2], Tyoyima J, Ayua[1], Gboyega A. Adebayo[2].

[1]Physics Unit, Department of Physical and Natural Sciences, University of The Gambia.

[2]Department of Physics, Federal University of Agriculture, Abeokuta P.M.B. 2240, Nigeria.

Ternary Half Heusler (HH) alloys are formed by combination of rock salt and zinc blend structure with a general formula of XYZ, where X and Y are transition metals with X being the most electropositive element and Z the main group elements with s, p valence electrons. These alloys can be semiconductors, half-metallic and metallic in nature. The band gap of these alloys are tunable by alloying wide indirect band gap materials with narrow direct band gap materials, making some of the HH desirable and suitable for spintronic and photovoltaic devices. The alloys used in this work are meant to be good candidates for spintronic devices. This study investigated the structural, electronic, magnetic, mechanical, and thermodynamic properties of HH alloys XCrSb (Y=Fe and Os) with 19 valence electron counts (VEC) as potential spintronic material using first principle calculations based on density functional theory (DFT) using *ab-initio* Quantum Espresso Simulation Package. The exchange-correlation energy was treated using generalized gradient approximation (GGA) with the Perdew, Burk and Ernzerhof parameterization while Thermo_pw code was used to calculate the mechanical and thermodynamic properties. The results obtained for the ferromagnetic state FeCrSb were in agreement with available theoretical and experimental results. Furthermore, the calculated electronic band structure and the total electronic density of states indicated half-metallic behaviour for both FeCrSb and OsCrSb alloys, with a minority-spin band gap of 1.40 and 0.94 eV, respectively. Finally, the obtained mechanical properties and phonon calculations predicted an anisotropic behaviour and dynamic stability of these alloys.

[1]   O.T. Uto, P.O. Adebambo, J.O. Akinlami, S. Kenmoe, G.A. Adebayo, Solids **3**, 22–33 (2022).

[2]   R. Gautier, X. Zhang, L. Hu, L. Yu, Y. Lin, T.O.L. Sunde, D. Chon, K.R. Poeppelmeier, A. Zunger, Nat. Chem. 7 (4) (2015) 308.

[3]   S. Wurmehl, G.H. Fecher, H.C. Kandpal, V. Kseno-fontov, C. Felser, H.J Lin, J. Morais, Phys. Rev. B **72**, 184434 (2005).

[4]   B.R.K. Nanda, J.I. Dasgupta, Phys. Condens. Matter **15**, 73077323 (2003).

[5]   A. Roy, J.W. Bennett, K.M. Rabe, D. Vanderbilt, Phys. Rev. Lett. **109**, 037602 (2012).