



United Nations
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ICTP - East African Institute
for Fundamental Research
under the auspices of UNESCO



Mini-African School on Electronic Structure Methods and Applications (MASESMA)

POSTER SESSION

Monday 11 November, 2019

Time: 18:00 HRS

Venue: Level 3 of ICTP-EAIFR Premises (EINSTEIN BLOCK) Former KIST2, College of Science and Technology University of Rwanda Nyarugenge Campus

- Structural, Electronic, Lattice dynamics, and Elastic properties of SnTiO_3 and PbTiO_3 using density functional theory
Shiferaw Gadisa Wollega University Ethiopia
- ELECTRON-PHONON INTERACTION, THERMAL AND MAGNETIC PROPERTIES IN POLAR GaAs NANOCRYSTAL UNDER ELECTROMAGNETIC FIELD
FOTUE ALAIN JERVE UNIVERSITY DE DSCHANG, CAMEROON CAMEROON
- STRUCTURAL AND ELECTRONIC PROPERTIES OF THE IRON Pnictide EuFe_2As_2 FROM FIRST PRINCIPLES.
NAOMY OMOGA KISII UNIVERSITY KENYA
- Titanium oxynitride with visible light photocatalysis capabilities
LYNET ALLAN UNIVERSITY OF NAIROBI KENYA
- Lawsone isomers, Lawsone Ether and Bilawsone for Dye-Sensitized Solar Cells Applications: DFT and UV-Vis studies
Amosi Makoye The Nelson Mandela African Institution of Science and Technology, Arusha, Tanzania Tanzania
- Ionic liquids based on 1-ethyl-3-methylimidazolium cation and anions of tetrafluoroborate and bis(trifluoromethylsulphonyl)imide: Structural and thermodynamic properties by DFT study
Plassidius Joachim Chengula Nelson Mandela African Institution of Science and Technology Tanzania

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- Pressure Effect on Structural Stability and Optical Absorption of Triclinic NbS₃ from DFT and Many-Body Perturbation calculations
Bonaventure Dusabe Institute of Mathematics and Physical Sciences (IMSP-Benin) Benin
- Structure of Electronically Reduced Zinc complexes : A survey of CASSCF and DFT results.
Berthelot Said Duvalier Ramlina Vamhindi University of Ngaoundere Cameroon
- INFORMATION PROCESSING AND THERMODYNAMIC PROPERTIES OF MICROTUBULES (MTs)
Christelle Ekosso University of Dschang Cameroon
- Hydration of L-glycylvaline and L-glycylvalylglycine zwitterions: Structural and vibrational studies using DFT method
Stève-Jonathan KOYAMBO-KONZAPA University of Bangui (CAR) Central Africa Republic (CAR)
- Computational study of charge transport in discharge products (NaO₂ and Na₂O₂) of Na-air battery
Natei Ermias Benti Addis Ababa University Ethiopia
- Ultrasensitive H₂S gas sensors based on p-type WS₂ hybrid materials
Georgies Alene Asres Addis Ababa Institute of Technology, Addis Ababa University Ethiopia
- STUDY OF ELECTRONIC AND STRUCTURAL PROPERTIES OF CADMIUM SULFIDE CdS IN ZINC- BLEND AND WURTZITE PHASE USING DENSITY FUNCTIONAL THEORY
Teshome Gerbaba Edossa Wollega University Ethiopia
- Optical Properties and Radiative Lifetimes of (Fe₂O₃)_n Clusters: A First Principles Approach
Henry Otunga Maseno University Kenya
- Charged domain walls at the PbTiO₃/PbTiO₃ interface
JAMES SIFUNA THE CATHOLIC UNIVERSITY OF EASTERN AFRICA KENYA
- First Principle study of the optoelectronic, thermal and mechanical properties of the quaternary diamond-like semiconductors Li₂ZnSnX₄ (X=S, Se, Te)
Felix Saouma Kaimosi Friends University College-Kenya Kenya
- Simulation of gravimetric capacity, structural and electronic of vanadium disulphide as anode material for lithium ion battery
Gloria Murila Masinde muliro university of science and technology Kenya
- Molecular Modeling of Porphyrin-based Photosensitizers for Water Purification using Density Functional Theory.
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- Computation of Transport Properties of Some Liquid Binary Alloys
Oluseyi Awe University of Ibadan, Ibadan, Nigeria Nigeria
- Theoretical prediction of thermodynamic activities of all components in liquid Ga-In-Tl and Ga-In-Tl-Zn
Olugbenga Oshakuade University of Ibadan, Ibadan, Nigeria Nigeria
- Relaxation methods for co-simulation of coupled circuit and finite element solvers
Nshimiyimana Jean de Dieu University of Rwanda Rwanda
- Spectroscopic and X-Ray Crystallography Characterization of Macro-molecule Schiff-Base ligands and Their Rhenium(I) Complexes
Gratien Habarurema University of Rwanda-College of Science and Technology Rwanda Rwanda
- Electronic properties of Perovskite thin film
Celline Awino Omondi Masinde Muliro University of science and technology Kenya
- Device Simulation of Sb2S3 Solar Cells by SCAPS-1D Software
Benjamin Victor Odari Ombwayo Masinde Muliro University of Science and Technology Kenya

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