

BOUAMRA Faiza
(Editor)

Abstracts of
1st International Conference on
Computational & Applied Physics

ICCAP'2021 (26th –28th September 2021)

Organized by

Surfaces, Interfaces and Thin Films Laboratory (LASICOM),
Department of Physics,
Faculty of Science,
University Saad Dahleb Blida 1,
Algeria

Published by

AIJR Publisher, Dhaurahra, Balrampur, India 271604



Table of Contents

Disclaimer.....	i
About the Conference	ix
Scientific Committee	xi
Acknowledgement	xii
The Superexchange Mechanism in Crystalline Compounds: The Case of KMF₃ (M=Mn, Fe, Co, Ni) Perovskites	1
Novel Visualization of Crystal Structure and Energetics	2
Ab Initio Calculation of Chirality in Crystals.....	3
Continuum Solvation for Finite and Infinite Periodic Systems in Crystal	4
Lattice Dynamics and Thermal Properties of Materials.....	5
Crystal17: A Modern Tool for Ab Initio Solid State Chemistry & Physics	6
Looking at Benchmarks for Density Functional Calculations	7
Understanding Structure and Properties of MgCl₂ Supported Ziegler-Natta Nanoclusters by DFT, Spectroscopy and Machine Learning: How Modelling Uncovers the Origin of Industrial Catalysis.....	8
Magnetism and Half-Metallicity of Solids from the Spin Polarization of P Orbitals.....	10
Enhanced Figure of Merit in Molecular Junctions	11
Intensity-based Wide-field Magneto-optical Microscopy	12
Boosting the Performance of Magnetic Nanoparticles: Magnetic Field-assistedAssembly and Magnetic Functionalization	13
Heterostructures Based on Functionalized Graphene and Free-standingGraphene Membranes.....	14
Effect of the Substrate on the Structural Properties of Cu₂ZnSnS₄ Thin FilmsSynthesized by Electrodeposition	15
Monte Carlo Method Study of Thin Films of The Spin-1 Ashkin Teller Model in the Presence of the Crystal Field	17
Dielectric Characterization by Impedance Meter of Thin Films Bi₂S_{3(0.6)}ZnS_(0.4) Composites	18

Green Synthesis and Characterization of Silver Nanoparticles	23
FEM Simulation and Performance Evaluation of MEMS Pressure Sensor Based onCapacitive Effect Using Molybdenum and Tungsten	25
Effect of Extended Gettering during the Emitter Formation on the ElectricalPerformance of Multicrystalline Silicon Based Solar Cells	27
Efficient Synthesis and Characterization of Highly Pure Nanosilica from Sand.....	29
Positron Annihilation Lifetime Spectroscopy in Neutrons Irradiated CR39 Polymer	31
Synthesis and Characterization of FeCo Nanoparticles by Hydrothermal Method.....	33
Microstructural Investigation of ZnO Nanowires for Therapeutic Applications	35
Real Time Ultrasoft Longitudinal Photons Self Energyat Next to-leading Order in Hot Scalar QED	36
Sensing Properties and Sensitivity Improvement of an Asymmetric Waveguide withDispersive Left-handed Material.....	40
Towards the Optimization of the Performance of N-I-P Microcrystalline Silicon nc-Si:H Flexible Solar Cells .	42
(2+1) D Massless Dirac Equation in Anti de-Sitter Space	44
Spin-polarized DFT Calculation of the Magneto-electronic Properties Under Pressure of the YCrSb Half-heusler Alloy.....	51
Mechanical Characteristics of Polyester Filled with Palm Fibers and Ash Particles.....	53
Superstatistical Properties of Ionization Rates of Li⁺.....	54
Raman and IR Spectroscopy of SnO₂ Nanostructures with Oxygen Vacancies: An Ab-Initio Calculations	57
Numerical Simulation of the Influence of an Sb layer on a Cu (In,Ga)Se₂ Solar CellsPerformance	60
Mechanical and Anisotropy Properties of SrCdPt Compound under Pressure	61
Effect of Annealing Time on Electrodeposited ZnS Thin Films	63
Effect of Electric and Magnetic Field on the Transport Coefficients of a Non-Equilibrium Gas by the Monte Carlo Method.....	65
Comparative Simulation of the Perovskite Solar Cell	68
Buckling Analysis of Carbon Nanotube-Reinforced Composite Plates Resting on ElasticFoundation	70
Study of n/p solar cell based on ITO/Si Heterojunction	71
Synthesis and Characterization of Layered Double Hydroxide Based on Zn and CrUsed for Anion Exchange .	73

Theoretical Study of the Structural Electronic Properties of half-Heusler RbInSn Alloy	74
Study of Microstructural and Electrical Properties of the (P)A-Si : H/(N)C-Si Heterojunction:Uncooled Microbolometer Application	75
DCF Method for Dispersion Compensation in Optical Fiber Link for LongHaul Communication.....	77
First-Principles Predictions of the Electronic, Optical and Thermoelectric Properties of the New Zintl-Phase Sr₂CdAs₂.....	78
Solvent Effect on Hyper-Rayleigh Scattering (HRS) First Hyperpolarizability of Substituted Polyene: Ab Initio Study	81
Ab-initio Investigation of Structural, Electronic and Topological Properties of Half- Heusler Compounds: TiRhz (Z=Sb,Bi).	83
Thermal And Dynamic Study of Confluent Round Jet of Different Diameters.....	86
First Principles Investigation of Structural and Electronic Properties of AlN/GaN Superlattices Growth Along Various Crystallographic Axes	88
Dangling Bonds Parameters Effect on Dark and Illuminated Conductivity in a-Si:H Absorber Layer for Solar Cells Applications.....	90
The Window Layer Doping Effect on the Performance of a SiO_x:H Based Solar Cells.....	92
Study of Ultra-Fast Phenomena Generated in Femtosecond Laser-material Interactions.....	95
Special Finite Element Modeling for Predicting the Mechanical Properties of CarbonNanotubes at the Atomic Scale	97
Improvement of Positron Annihilation Lifetime Spectrometer Resolution: AComparative Study.....	98
Thermal Properties of the Klein-Gordon Oscillator in Deformed Space.....	100
Role of Hydroxyl Group in CO Adsorption on SnO₂ (110) Surface Investigated by a First-principle Study	102
The Effect of Aluminum Sources On (Gd_{0.7}Lu_{0.3})₃Al₅O₁₂ Cubic Garnet Structure Synthesized by Co Precipitation Method	104
Structure Properties of LiAl (WO₄)₂ Solid Solution	106
The Influence of Preparation Parameters on Structural and Optical Properties of n-Type Porous Silicon.....	108
Study the Structural Properties of WO₃:Fe Thin FilmsElaborated by Spray Pyrolysis Technique at 450 °C....	110
Calculation of the Structural Properties of GdB₃O₃ by the Theoretical Method ab-initio.....	111
Computational Determination of theMagneto-electronic Properties of Ce_{1-x}Cu_xO₂ (x=12.5%): Emerging Materials for Spintronic Devices.....	113

First-Principles Calculations of Structural, Elastic, and Electronic Properties of Antiperovskites Ca_3SiO and Ca_3GeO	115
Hyperfine Structures ab-initio Calculations of the $2\text{p}^4(^3\text{P})3\text{d}^{2S+1}\text{L}_1$ States in the Fluorine Atom	117
Synthesis of Zeolites from Pure and Natural Products, Modification and Application in Wastewater Treatment	119
Characterization (FT-Raman, FT-II Spectra) of 3,5-Dimethoxybenzaldehyde $\text{C}_9\text{H}_{10}\text{O}_3$ and Compared with Density Functional Theory (DFT)	121
Cathodoluminescence Calculation of AlGaN/GaN Quantum-Wells by MonteCarlo Model: Effect of Compositional and Temperature	123
Bloch Surface Waves Based Biosensor Using a Ternary Photonic Crystal	126
Hyperfine Structure of the $3\text{p}^44\text{s}~^4\text{p}$ State of the Chlorine Atom.....	128
First-principles Calculations of the Physical Properties and Stability of ScN	130
Surface Metal Effect on I(V) Characteristics Ti/6H-Sic Schottky Diode at RoomTemperature	133
Adsorption of Anticancer Drug Molecule on Single Wall Carbon Nanotube: An ab-initio Study.....	135
First Principal Study of Physical Properties of Rare Earth Based Heusler Compounds X_2RuPb ($\text{X}=\text{Sc, Y and La}$)	137
Elaboration and Characterization of Black Silicon for Photovoltaic Solar Cells	139
Structural Investigations Studies of Antimony-Tungsten and Sodium Metaphosphate Glass Systems with NaPO_3 as Additive.....	141
In-depth Analyses of P-type Silicon Solar Cells by Laser-Induced Breakdown Spectroscopy (LIBS).....	144
Diagnosis of an Unknown Solar Cell by Electrical Characterization	146
Affecting Parameters on Polymers Surface Treatment by Atmospheric Pressure Plasma Jets	148
Crystal Structure and Comparative Study via Hirshfeld Surface Analyses of Charge Transfer Compounds Based on Anthranilic Acid.....	150
Effect of Various Auxiliary Acceptors on the Optical and Photovoltaic Properties of a D-A'-π-A Sensitizing Dye. DFT and TD-DFT Study	152
Preparation and Characterizations of MgFe_2O_4 Spinel Semiconductor.....	153
Numerical Thickness Optimization Study of CIGS Based Solar Cells with SCAPS-1D.....	155
Influence of Porosity on the Structural and Electronic Properties of Porous Silicon	157

Label-free Biosensor Based on Photonic Crystal Microcavity for MalariaDetection with High Sensitivity	159
Ab-Initio Study of the Ferromagnetic Half-Metallic Perovskite KMgO₃.....	161
Ab Initio Calculations of the Structural and Electronics Properties of DoubleTungstates NaY(WO₄)₂.....	164
First-principles Study of Structural, Electronic, Elastic and Thermal Propertiesof XBPd₃ (X = Ca, Mg)	166
Synthesis and Characterization of Polystyrene (PS)/Copper Oxide CuO Nanocomposites.....	167
Theoretical Study of Structural and Electronics Properties of Lithium Niobate LiNbO₃	169
Effect of Doping with Niobium on the Properties of Titanium Dioxide Thin FilmsPrepared by Sol Gel (Spin-coating) Process	171
Structural, Electronic, Elastic and Thermodynamic Properties of ReAuSn	174
Investigation of Deposition Temperature and Time Effect on the Quality of FSF in n-PERT Solar Cells Using Phosphorus Doped Paper Sheets.....	177
Ab-initio Study of the Optoelectronic Properties of CsXCl₃ Perovskites (X = Pb, Sn or Ge).....	179
High Spin Polarization and Mechanic Stability of Half-Heusler Compounds: CrFeSn and CrFeGe as a Candidate in the Spin-FETs for Spintronic Applications.....	180
Investigation of an Additional Oxidation in-situ Step During Boron Diffusion Processes on P⁺ Emitter Properties.....	182
Effect of Heat Treatment on Structural and FTIR and Lowercase	183
Characterization of Interfacial and Mechanical Properties Between Fiber and Polymer Matrix in Composite Materials	186