Year of Publication	Research Title	Researcher Name	Name of Research group
2019	Structural, electronic, magnetic, optical and thermoelectric response of half-metallic AMnTe(2) (A = Li, Na, K): An ab-initio calculations		
2019	Electronic structures and optical spectroscopies of 3d-transition metals-doped melanin for spintronic devices application		
2019	Voltage-controllable multifunctional spin polarizer based on side-coupled quantum dots		
2019	Exploring the opto-electronic and charge transfer nature of F-BODIPY derivatives at molecular level: A theoretical perspective		
2019	The systematic study of mechanical, thermoelectric and optical properties of lead based halides by first principle approach		
2019	Theoretical investigation of thermodynamic and optoelectronic properties of Ce4+ doped SrZrO3 ceramics: A DFT study		
2019	DFT prediction of the structural, electronic, thermoelectric and optical properties of ternary pnictides MgBe2X2 (X = N, P, As, Sb, Bi): A novel analysis of beryllium with 2A-and 5B-Elements of the structure type CaAl2Si2		
2019	Optoelectronic properties of new direct bandgap polymorphs of single-layered Germanium sulfide		
2019	Engineering of the band gap and optical properties of InxGa1-x(As/Sb) via across composition alloying for solar cell applications using density functional theory-based approaches		
2019	Impact of phosphorous and sulphur substitution on Dirac cone modification and optical behaviors of monolayer graphene for nano-electronic devices		
2019	Exploring the origin of p-type half-metallic ferromagnetism in beryllium doped alkali based perovskites		
2019	Effect of extended alkyl auxiliary groups on optical and electronic properties of Benzo[2,1-b:3,4-b ':5,6-c ']trithiophene derivatives at bulk level: a first-principles study		

2019	Comprehensive study of the physical properties of Ba(3)Pn(2) (Pn=N, P, As, Sb and Bi) through first principles technique
2019	Physical properties of alkali metals-based iodides via Ab-initio calculations
2019	Half-metallic ferromagnetism and optical behavior in alkaline-earth metals based Beryllium perovskites: DFT calculations
2019	Dimensionality reduction of germanium selenide for high-efficiency thermoelectric applications
2019	High spin polarization in formamidinium transition metal iodides: first principles prediction of novel half-metals and spin gapless semiconductors
2019	Exploring Novel Flat-Band Polymorphs of Single-Layered Germanium Sulfide for High-Efficiency Thermoelectric Applications
2019	Systematic Investigation of the Electrochemical Properties of Natural Melanin for Various Electrode Cells
2019	The study of mechanical and thermoelectric behavior of MgXO3 (X = Si, Ge, Sn) for energy applications by DFT
2019	Theoretical prediction of optoelectronic and thermoelectric properties of RbXO2 (X = Al, Ga, In) for renewable energy applications
2019	Ab-initio investigations of structural, optoelectronic and thermoelectric properties of AIn(2)Se(4) (A = Zn, Cd) spinels
2019	First-principles calculations of electronic and magnetic properties of XMn2Y2 (X = Ca, Sr; Y = Sb, Bi) compounds
2019	The doping effect of Fe, Cu and Zn ions on the structural and electrochemical properties and the thermostability of natural melanin extracted from Nigella sativa L
2019	Control of optical absorption and fluorescence spectroscopies of natural melanin at different solution concentrations
2019	Investigations of the optoelectronic properties of novel polymorphs of single-layered Tin-Sulfide for nanoscale optoelectronic and photovoltaic applications
2019	Exploring the functional properties of Trimethoxy-Phenylpyridine as efficient optical and nonlinear optical material: A quantum chemical approach
2019	Optoelectronic pressure dependent study of MgZrO3 oxide and ground state thermoelectric response using Ab-initio calculations

2019	Structural, electronic, elastic, magnetic and optical properties of binary intermetallic compounds AB(3) (A = Si, Ge, Sn and B = Cr, V, Nb)
2019	First-Principles Investigation of Structural, Electronic, Optical, and Magnetic Properties of Ternary Mixed Compound CsTexS1-x
2019	Effects of Stone-Wales Defect on the Electronic and Optical Properties of Armchair MoS2 Nanoribbon: First-Principles Calculations
2019	Relativistic effects on the electronic and optical characteristics of Cd1-xHgxTe alloys-based solar cell materials
2019	Strain effects on structural, electronic, and optical properties of BeO by DFT
2019	Electronic, and thermoelectric properties of half-heusler compounds MCoSb (M = Ti, Zr, Hf): a first principles study
2019	Investigation of the structural, electrical, optical and magnetic properties of XMg4Mn6O15 (X = K, Rb, and Cs) compounds
2019	First-principles analysis for the modulation of energy band gap and optical characteristics in HgTe/CdTe superlattices
2019	Investigations of physical aspects of spinel ABi(2)O(4) (A=Zn, Cd) oxides via ab-initio calculations
2019	First-principle simulations of XIn2S4 (X = Zn, Cd) thiospinels for energy harvesting devices
2019	The Theoretical Investigation of Electronic, Magnetic, and Thermoelectric Behavior of LiZ(2)O(4) (Z = Mn, Fe, Co, and Ni) by Modified Becke and Johnson Approach
2019	Highly absorbent cubic structured Silicon-monochalcogenides: Promising materials for photovoltaic applications
2019	Electronic and magnetic properties of alkali metal chlorides A(2)MCl(6) (A =K, Rb, Cs; M =Mn, Mo): A density functional theory study
2019	First principles study of RbVF3: A spin gapless semiconductor under high pressure
2019	Effects of anion replacement on the physical properties of CaCd2X2 (X = P, As, Sb, Bi)
2019	The first-principle study of mechanical, optoelectronic and thermoelectric properties of CsGeBr3 and CsSnBr3 perovskites

2019	Density Functional Theory Evaluation of Ceramics Suitable for Hybrid Advanced Oxidation Processes: A Case Study for Ce4+-Doped BaZrO3
2019	A theoretical analysis of elastic and optical properties of half Heusler MCoSb (M = Ti, Zr and Hf)
2019	Electronic structure, optical and thermoelectric properties of CaMgSi1-xCx (x=0, 0.5): an ab-initio study
2019	Design and characterization of novel polymorphs of single-layered tin-sulfide for direction-dependent thermoelectric applications using first-principles approaches
2019	Lattice dynamics, mechanical stability and electronic structure of Fe-based Heusler semiconductors
2019	Full Heusler alloys (Co2TaSi and Co2TaGe) as potential spintronic materials with tunable band profiles
2019	Structural, electronic and optical properties of furan based materials at bulk level for photovoltaic applications: A first-principles study
2019	Impact of fluorine on organic cation for determining the electronic and optical properties of CH3-xFxNH3PbI3 (x=0, 1, 2, 3) hybrid perovskites-based photovoltaic devices
2019	Electronic and optical behaviors of methylammonium and formamidinium lead trihalide perovskite materials
2019	Graphene Oxide Nanoscrolls: Synthesis, Characterization, Optical, and Electrical Properties
2018	First-principles investigation of the electronic band structures and optical properties of quaternary ABaMQ(4) (A = Rb, Cs; M = P, V; and Q = S) metal chalcogenides
2018	First principles study of electronic structures of Cd-0.9375 Co-0.0625 X (X = S, Se, Te) for magnetic, optical and thermoelectric device applications
2018	Effects of Multiple Stacking Faults on the Electronic and Optical Properties of Armchair MoS2 Nanoribbons: First- Principles Calculations
2018	The pressure-induced indirect to direct bandgap transition and thermoelectric response in SrTiO3: An ab-initio study
2018	Thermoelectric properties of the novel cubic structured silicon monochalcogenides: A first-principles study

2018	Ab Initio Study of Electronic, Magnetic, and Thermoelectric Response of ZTi(2)O(4) (Z = Mg, Zn, and Cd) Through mBJ Potential
2018	Systematic DFT study of the impact of anionic variations on the physical properties of Cd1-xMnxX (X=S, Se, Te; x=6.25%)
2018	Investigations of half-metallic ferromagnetism and thermoelectric properties of cubic XCrO3 (X = Ca, Sr, Ba) compounds via first-principles approaches
2018	Predicting the electronic structure, magnetism, and transport properties of new Co-based Heusler alloys
2018	Monte Carlo Simulation of Photon Transport for Computing Fluence Rate in Biological Tissue
2018	Structural, Optoelectronic and Thermoelectric Properties of Ternary CaBe2X2 (X = N, P, As, Sb, Bi) Compounds
2018	DFT understandings of structural properties, mechanical stability and thermodynamic properties of BaCfO3 perovskite
2018	Ab-initio prediction of structural, electronic and magnetic properties of Hexafluoromanganete(IV) complexes
2018	Electronic Properties of Armchair MoS2 Nanoribbons with Stacking Faults: First-Principles Calculations
2018	Physical properties of cubic BaGeO3 perovskite at various pressure using first-principle calculations for energy renewable devices
2018	Spin-induced transition metal (TM) doped SnO2 a dilute magnetic semiconductor (DMS): A first principles study
2018	Mono and bi-layer germanene as prospective anode material for Li-ion batteries: A first-principles study
2018	Study of optoelectronic and thermoelectric properties of BaSiO3 perovskite under moderate pressure for energy renewable devices applications
2018	Physical properties of half-Heusler YMnZ (Z = Si, Ge, Sn) compounds via ab-initio study
2018	The pressure-induced mechanical and optoelectronic behavior of cubic perovskite PbSnO3 via ab-initio investigations
2018	Electronic band profiles and optical response of Cd3Y2 (Y = N, P and As) compounds

2018	Impact of anion replacement on the optoelectronic and thermoelectric properties of CaMg2X2, X= (N, P, As, Sb, Bi) compounds
2018	Anion-Cation Replacement Effect on the Structural and Optoelectronic Properties of the LiMX2 (M =Al, Ga, In; X=S, Se, Te) Compounds: A First Principles Study
2018	Ab-initio study of thermodynamic stability, thermoelectric and optical properties of perovskites ATiO(3) (A=Pb, Sn)
2018	Electronic Structure, Optical and Transport Properties of Double Perovskite La2NbMnO6: A Theoretical Understanding from DFT Calculations
2018	Structural and electronic properties of 90 degrees dislocations in silicon nanorods: A first-principles calculation
2018	First principles study of ferromagnetism, optical and thermoelectric behaviours of AVO(3) (A = Ca, Sr, Ba) perovskites
2018	Electronic structure, mechanical and thermodynamic properties of BaPaO3 under pressure
2018	Ab-initio study of electronic, magnetic and thermoelectric behaviors of LiV2O4 and LiCr2O4 using modified Becke-Johson (mBJ) potential
2018	Engineering the electronic band structures of novel cubic structured germanium monochalcogenides for thermoelectric applications
2018	Physical properties of half-metallic AMnO(3) (A = Mg, Ca) oxides via ab initio calculations
2018	The effect of replacing pnictogen elements on the physical properties of SrMg2X2 (X = N, P, As, Sb, Bi) Zintl compounds
2018	Effect of Varying Pnictogen Elements (Pn = N, P, As, Sb, Bi) on the Optoelectronic Properties of SrZn2 Pn(2)
2018	First principles examination of electronic structure and optical features of 4H-GaN1-xPx polytype alloys
2018	Electronic, optical and thermoelectric properties of SnGa2GeX6 (X = S, Se) compounds
2018	Theoretical Investigation of Half-Metallic Oxides XFeO3 (X = Sr, Ba) via Modified Becke-Johnson Potential Scheme
2018	Exploring single-layered SnSe honeycomb polymorphs for optoelectronic and photovoltaic applications

2018	Exploring thermoelectric materials for renewable energy applications: The case of highly mismatched alloys based on AlBi1-xSbx and InBi1-xSbx		
2018	Optoelectronic and transport properties of LiBZ (B = Al, In, Ga and Z = Si, Ge, Sn) semiconductors		
2018	A case study of Fe(2)TaZ (Z = Al, Ga, In) Heusler alloys: hunt for half-metallic behavior and thermoelectricity		
2018	A new cryptography algorithm for quantum images		
2018	Systematic studies of the structural and optoelectronic characteristics of CaZn2X2 (X = N, P, As, Sb, Bi)		
2018	Systematic study of elastic, electronic, optical and thermoelectric properties of cubic BiBO3 and BiAlO3 compounds at different pressure by using ab-initio calculations		
2017	Effect of gold nanoparticles on radiation doses in tumor treatment: a Monte Carlo study		
2017	Suppressed Kondo effect and Kosterlitz-Thouless-type phase transition induced by level difference in a triple dot device		
2017	Voltage-controlled Kosterlitz-Thouless transitions and various kinds of Kondo behaviors in a triple dot device		
2017	Ab Initio Investigation of the Structural and Electronic Properties of HgTe/CdTe Superlattices		
2017	Ab-Initio Investigations of Magnetic Properties and Induced Half-Metallicity in Ga1-xMnxP (x=0.03, 0.25, 0.5, and 0.75) Alloys		
2017	Compositional and spin-orbit control on the electronic structure and optical characteristics of ZnHgTe alloys using mBJ-GGA approach		
2017	Quantum confinement effect on the electronic and optical features of InGaN-based solar cells with InGaN/GaN superlattices as the absorption layers		
ORCID	https://orcid.org/0000-0002-1679-9406		

2017	Structural Study of SrTiO3 Doped with Mn Using X-Ray Diffraction	Dr. Zainab boq	
2017	Enhancement of external quantum efficiency and quality of heterojunction white LEDs by varying the size of ZnO nanorods	Dr. Sausan Sawaf	
2019	Dose-dependent cytotoxicity of polyethylene glycol loaded nano-graphene oxide in cultured cerebral cortical cells	Dr. Abeer Alshammari	
2019	Study of a saturation point to establish the doping density limit of silicon with graphene oxide		
2018	Effect of solvents on optical band gap of silicon-doped graphene oxide		
2017	Enhancement of external quantum efficiency and quality of heterojunction white LEDs by varying the size of ZnO nanorods		
ORCID	https://orcid.org/0000-0002-9571-8060		
2019	Effect of secondary phases on the thermoelectric properties of Zn2GeO4 nano-crystals grown by thermal evaporation on Au coated Si substrate		
2019	A two step technique to remove the secondary phases in CZTS thin films grown by sol - gel method		

2019	Study of a saturation point to establish the doping density limit of silicon with graphene oxide	Dr. Narjes Panu	
2019	Tailoring the thermoelectric properties of sol-gel grown CZTS/ITO thin films by controlling the secondary phases		
2019	Enhancing external quantum efficiency and luminescence quality of ZnO nanorods based Schottky LEDs by Mg doping		
2019	Exploring the fluorescence properties of reduced graphene oxide with tunable device performance		
2018	Solution processable inverted structure ZnO-organic hybrid heterojuction white LEDs		
2018	ZnMgO-nanorod-based Schottky Light-emitting Diode Fabricated on n-SiC Substrate Using Low-temperature Method		
2017	Enhancement of external quantum efficiency and quality of heterojunction white LEDs by varying the size of ZnO nanorods		
ORCID	http://orcid.org/0000-0003-1007-9683		