

| سنة نشر البحث | عنوان البحث | اسم الباحثة | اسم المجموعة البحثية |
|------------------|---|--------------|----------------------------|
| 2019 | Structural, electronic, magnetic, optical and thermoelectric response of half-metallic AMnTe(2) (A = Li, Na, K): An ab-initio calculations | أ. د. أمل د. | |
| 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 Ce ⁴⁺ doped SrZrO ₃ ceramics: A DFT study | | |
| 2019 | DFT prediction of the structural, electronic, thermoelectric and optical properties of ternary pnictides MgBe ₂ X ₂ (X = N, P, As, Sb, Bi): A novel analysis of beryllium with 2A-and 5B-Elements of the structure type CaAl ₂ Si ₂ | | |
| 2019 | Optoelectronic properties of new direct bandgap polymorphs of single-layered Germanium sulfide | | |
| 2019 | Engineering of the band gap and optical properties of In _x Ga _{1-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 | | |

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| 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 MgXO ₃ (X = Si, Ge, Sn) for energy applications by DFT |
| 2019 | Theoretical prediction of optoelectronic and thermoelectric properties of RbXO ₂ (X = Al, Ga, In) for renewable energy applications |
| 2019 | Ab-initio investigations of structural, optoelectronic and thermoelectric properties of Aln(2)Se(4) (A = Zn, Cd) spinels |
| 2019 | First-principles calculations of electronic and magnetic properties of XMn ₂ Y ₂ (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 MgZrO ₃ oxide and ground state thermoelectric response using Ab-initio calculations |

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| 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-xHg _x Te 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 XMg ₄ Mn ₆ O ₁₅ (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 XIn ₂ S ₄ (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 RbVF ₃ : A spin gapless semiconductor under high pressure |
| 2019 | Effects of anion replacement on the physical properties of CaCd ₂ X ₂ (X = P, As, Sb, Bi) |
| 2019 | The first-principle study of mechanical, optoelectronic and thermoelectric properties of CsGeBr ₃ and CsSnBr ₃ perovskites |

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| 2019 | Density Functional Theory Evaluation of Ceramics Suitable for Hybrid Advanced Oxidation Processes: A Case Study for Ce ⁴⁺ -Doped BaZrO ₃ |
| 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 CaMgSi _{1-x} C _x (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 (Co ₂ TaSi and Co ₂ TaGe) 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 CH _{3-x} F _x NH ₃ PbI ₃ (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 MoS ₂ Nanoribbons: First- Principles Calculations |
| 2018 | The pressure-induced indirect to direct bandgap transition and thermoelectric response in SrTiO ₃ : An ab-initio study |
| 2018 | Thermoelectric properties of the novel cubic structured silicon monochalcogenides: A first-principles study |

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| 2018 | Ab Initio Study of Electronic, Magnetic, and Thermoelectric Response of $ZTi(2)O(4)$ ($Z = Mg, Zn, \text{ and } Cd$) Through mBJ Potential |
| 2018 | Systematic DFT study of the impact of anionic variations on the physical properties of $Cd_{1-x}Mn_xX$ ($X=S, Se, Te; x=6.25\%$) |
| 2018 | Investigations of half-metallic ferromagnetism and thermoelectric properties of cubic $XCrO_3$ ($X = Ca, Sr, Ba$) 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 $CaBe_2X_2$ ($X = N, P, As, Sb, Bi$) Compounds |
| 2018 | DFT understandings of structural properties, mechanical stability and thermodynamic properties of $BaCfO_3$ perovskite |
| 2018 | Ab-initio prediction of structural, electronic and magnetic properties of Hexafluoromanganate(IV) complexes |
| 2018 | Electronic Properties of Armchair MoS_2 Nanoribbons with Stacking Faults: First-Principles Calculations |
| 2018 | Physical properties of cubic $BaGeO_3$ perovskite at various pressure using first-principle calculations for energy renewable devices |
| 2018 | Spin-induced transition metal (TM) doped SnO_2 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 $BaSiO_3$ 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 $PbSnO_3$ via ab-initio investigations |
| 2018 | Electronic band profiles and optical response of Cd_3Y_2 ($Y = N, P \text{ and } As$) compounds |

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| 2018 | Impact of anion replacement on the optoelectronic and thermoelectric properties of CaMg_2X_2 , $\text{X} = (\text{N}, \text{P}, \text{As}, \text{Sb}, \text{Bi})$ compounds |
| 2018 | Anion-Cation Replacement Effect on the Structural and Optoelectronic Properties of the LiMX_2 ($\text{M} = \text{Al}, \text{Ga}, \text{In}$; $\text{X} = \text{S}, \text{Se}, \text{Te}$) Compounds: A First Principles Study |
| 2018 | Ab-initio study of thermodynamic stability, thermoelectric and optical properties of perovskites ATiO_3 ($\text{A} = \text{Pb}, \text{Sn}$) |
| 2018 | Electronic Structure, Optical and Transport Properties of Double Perovskite $\text{La}_2\text{NbMnO}_6$: 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 ($\text{A} = \text{Ca}, \text{Sr}, \text{Ba}$) perovskites |
| 2018 | Electronic structure, mechanical and thermodynamic properties of BaPaO_3 under pressure |
| 2018 | Ab-initio study of electronic, magnetic and thermoelectric behaviors of LiV_2O_4 and LiCr_2O_4 using modified Becke-Johnson (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 ($\text{A} = \text{Mg}, \text{Ca}$) oxides via ab initio calculations |
| 2018 | The effect of replacing pnictogen elements on the physical properties of SrMg_2X_2 ($\text{X} = \text{N}, \text{P}, \text{As}, \text{Sb}, \text{Bi}$) Zintl compounds |
| 2018 | Effect of Varying Pnictogen Elements ($\text{Pn} = \text{N}, \text{P}, \text{As}, \text{Sb}, \text{Bi}$) on the Optoelectronic Properties of SrZn_2Pn_2 |
| 2018 | First principles examination of electronic structure and optical features of $4\text{H-GaN}_{1-x}\text{Px}$ polytype alloys |
| 2018 | Electronic, optical and thermoelectric properties of $\text{SnGa}_2\text{GeX}_6$ ($\text{X} = \text{S}, \text{Se}$) compounds |
| 2018 | Theoretical Investigation of Half-Metallic Oxides XFeO_3 ($\text{X} = \text{Sr}, \text{Ba}$) via Modified Becke-Johnson Potential Scheme |
| 2018 | Exploring single-layered SnSe honeycomb polymorphs for optoelectronic and photovoltaic applications |

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| 2018 | Exploring thermoelectric materials for renewable energy applications: The case of highly mismatched alloys based on $\text{AlBi}_{1-x}\text{Sbx}$ and $\text{InBi}_{1-x}\text{Sbx}$ | آمال لعارف | |
| 2018 | Optoelectronic and transport properties of LiBZ ($\text{B} = \text{Al, In, Ga}$ and $\text{Z} = \text{Si, Ge, Sn}$) semiconductors | | |
| 2018 | A case study of Fe(2)TaZ ($\text{Z} = \text{Al, Ga, In}$) 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 CaZn_2X_2 ($\text{X} = \text{N, P, As, Sb, Bi}$) | | |
| 2018 | Systematic study of elastic, electronic, optical and thermoelectric properties of cubic BiBO_3 and BiAlO_3 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 $\text{Ga}_{1-x}\text{MnxP}$ ($x=0.03, 0.25, 0.5, \text{ and } 0.75$) 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 SrTiO_3 Doped with Mn Using X-Ray Diffraction | د. زينب بوق | |

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| 2017 | Enhancement of external quantum efficiency and quality of heterojunction white LEDs by varying the size of ZnO nanorods | د. سوسن الصواف | |
| 2019 | Dose-dependent cytotoxicity of polyethylene glycol loaded nano-graphene oxide in cultured cerebral cortical cells | د. عبير الشمري | |
| 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 Zn ₂ GeO ₄ nano-crystals grown by thermal evaporation on Au coated Si substrate | د. نرجس بانو | |
| 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 | | |
| 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 heterojunction white LEDs | | |

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| 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 | |