# Sikander Azam

List of Publications by Year
in descending order



| 121 | 1,204 | 471509 | 610901 |
|---|---|---|---|
| papers | citations | 17 h-index | 24 g-index |

| 124 | 124 | 124 | 828 |
|---|---|---|---|
| all docs | docs citations | times ranked | citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | Insight into the Structural, Magneto-electronic, and Mechanical Characteristic of Y2MnZ (Zâ€‰=â€‰Al, Ga,) Tj ETQq1 1 0.784314 rgB | 1.8 | 5 |
| 2 | The effect of substitutional doping of Yb<sup>2+</sup> on structural, electronic, and optical properties of CsCaX <sub>3</sub> (X: Cl, Br, I) phosphors: a first-principles study. Journal of Physics Condensed Matter, 2022, 34, 065502. | 1.8 | 4 |
| 3 | Effects of Mn2+ doping on the electronic, structural, and optical properties of Cs2ZrF6: An ab initio study. Journal of Physics and Chemistry of Solids, 2022, 162, 110492. | 4.0 | 4 |
| 4 | First-principles study of opto-electronic and thermoelectric properties of SrCdSnX4 (X=S, Se, Te) alkali metal chalcogenides. Computational Condensed Matter, 2022, 30, e00625. | 2.1 | 17 |
| 5 | Optoelectronic investigation of lithium di-manganese oxide with doping of Nickel via Li1-xNixMn2O4 where X= 4 % and 8% composition and their application. Journal of Solid State Chemistry, 2022, 309, 122918. | 2.9 | 1 |
| 6 | On the role of Zn doping on tuning the electronic and optical properties of MnCr<sub>2</sub>O<sub>4</sub> spinel via Mn<sub>0.5</sub>Zn<sub>0.5</sub>Cr<sub>2</sub>O<sub>4</sub> doping scheme: A first-principles quantum computational analysis. Physica Scripta, 2022, 97, 045812. | 2.5 | 3 |
| 7 | Optoelectronic features of NbCu3Q4 (Q = S, Se) for p-type transparent conducting application: DFT and HSE06. Optik, 2022, 262, 169297. | 2.9 | 3 |
| 8 | First-principles investigations of metal chalcogenides Tl2Hg3X4(X=S,Se,Te) for advanced optoelectronic and thermoelectric applications. Journal of Solid State Chemistry, 2022, 312, 123199. | 2.9 | 15 |
| 9 | Density functional theory-based quantum-computational analysis on the strain-assisted phononic, electronic, photocatalytic properties and thermoelectric performance of monolayer Janus SnSSe. Applied Physics A: Materials Science and Processing, 2022, 128, . | 2.3 | 3 |
| 10 | Optoelectronic properties of Nd3+ doped CaTa2O6: Insights from the GGAâ€‰+â€‰U calculations. Optik, 2021, 225, 165270. | 2.9 | 4 |
| 11 | Mechanical and thermodynamic stability, structural, electronics and magnetic properties of new ternary thorium-phosphide silicides ThSixP1-x: First-principles investigation and prospects for clean nuclear energy applications. Nuclear Engineering and Technology, 2021, 53, 592-602. | 2.3 | 11 |
| 12 | Insight into electronic and optical properties of Eu+2-doped CaTiO3 from GGA+U calculations. Journal of Solid State Chemistry, 2021, 293, 121796. | 2.9 | 4 |
| 13 | Investigation of structural, electronic and optical properties of potassium and lithium based ternary Selenoindate: Using first principles approach. Journal of Solid State Chemistry, 2021, 293, 121778. | 2.9 | 42 |
| 14 | Rb and Cs doping effects in sodium borohydride: Density functional theory for hydrogen (H2) storage purpose. International Journal of Hydrogen Energy, 2021, 46, 2405-2412. | 7.1 | 4 |
| 15 | Insight view of Hf2CrZ (ZÂ= B, Ga, In, Si, Ge, Sn) Heusler materials via DFT calculations: A study on structural, electronic and magnetic properties. Computational Condensed Matter, 2021, 26, e00518. | 2.1 | 4 |
| 16 | First principle approach to substitutional effect of europium (Eu+2) on electronic and optical parameters of strontium pyroniobate for low temperature applications. Journal of Alloys and Compounds, 2021, 854, 157115. | 5.5 | 5 |
| 17 | Proposal of new stable <scp> ABC <sub>2</sub> </scp> type ternary semiconductor pnictides <scp> K <sub>3</sub> Cu <sub>3</sub> P <sub>2</sub> </scp> and <scp> K <sub>3</sub> Ni <sub>3</sub> P <sub>2</sub> </scp>. International Journal of Energy Research, 2021, 45, 2980-2996. | 4.5 | 10 |
| 18 | Structure stability, half metallic ferromagnetism, magneto-electronic and thermoelectric properties of new zintl XCr2Bi2 (X=Ca, Sr) compounds for spintronic and renewable energy applications. Physica B: Condensed Matter, 2021, 607, 412866. | 2.7 | 21 |

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|---|---|---|---|
| 19 | Exploring fundamental properties of Mg 0. 915 A 0 . 085 H 2 (AÂ=ÂTi, Fe) for potential hydrogen storage application: Firstâ€principles study. International Journal of Energy Research, 2021, 45, 14971-14984. | 4.5 | 2 |
| 20 | Structural, electronic, optical and thermodynamical properties of Cu3Se2 and [Cu3Se2]:Zn compounds: Using DFT. Journal of Solid State Chemistry, 2021, 298, 122125. | 2.9 | 4 |
| 21 | Electronic band structure and optical characteristic of silver lanthanide XAgSe2 (XÂ=ÂEu and Er) dichalcogenides: Insight from DFT computations. Inorganic Chemistry Communication, 2021, 129, 108586. | 3.9 | 2 |
| 22 | Effect of Nb, Ta and V replacements on electronic, optical and elastic properties of NbCu3Se4: A GGA+U study. Journal of Solid State Chemistry, 2021, 301, 122338. | 2.9 | 18 |
| 23 | Effect of manganese on electronic and optical properties of Ba2ZnS3: A DFT study. Journal of Solid State Chemistry, 2021, 301, 122335. | 2.9 | 9 |
| 24 | Synthesis and Fabrication of Co1â^'xNixCr2O4 Chromate Nanoparticles and the Effect of Ni Concentration on Their Bandgap, Structure, and Optical Properties. Journal of Composites Science, 2021, 5, 247. | 3.0 | 7 |
| 25 | First-principles calculations of structural, electronic, magnetic, thermoelectric, and thermodynamic properties of BaMn2P2 in the Anti and ferromagnetic phase. Journal of Solid State Chemistry, 2021, 302, 122388. | 2.9 | 14 |
| 26 | A systematic study on optoelectronic properties of Mn<sup>4+</sup>-activated Zr-based hexafluoride red phosphors X<sub>2</sub>ZrF<sub>6</sub> (XÂ=ÂK, Na, Cs): first-principles investigation and prospects for warm-white LEDs applications. Physica Scripta, 2021, 96, 015801. | 2.5 | 10 |
| 27 | An ab-initio investigation of the electronic structure, chemical bonding and optical properties of Ba<sub>2</sub>HgS<sub>5</sub> semiconductor. Molecular Physics, 2020, 118, e1587026. | 1.7 | 5 |
| 28 | Electronic, optical and thermoelectric properties of new metal-rich homological selenides with palladiumâ€"indium: Density functional theory and Boltzmann transport model. Journal of Physics and Chemistry of Solids, 2020, 138, 109229. | 4.0 | 18 |
| 29 | DFT modeling of thermoelectric and optical features of novel MgxSn1-xSe (xÂ= 6%, 12% & 18%). Journal of Molecular Graphics and Modelling, 2020, 94, 107484. | 2.4 | 6 |
| 30 | Cation effect on electronic, optical and thermoelectric properties of perovskite oxynitrides: Density functional theory. Materials Science in Semiconductor Processing, 2020, 107, 104800. | 4.0 | 6 |
| 31 | Electronic, elastic, thermodynamic and vibrational properties of Li6BeZrF12: Insights from DFT-based computer simulation. Computational Condensed Matter, 2020, 25, e00506. | 2.1 | 2 |
| 32 | Effect of Coulomb interactions on optoelectronic properties of Eu doped lanthanide stannates pyrochlore: DFTÂâ€‹+Ââ€‹U investigations. Journal of Solid State Chemistry, 2020, 290, 121522. | 2.9 | 5 |
| 33 | Proposal of new spinel oxides semiconductors ZnGaO2, [ZnGaO2]:Mn3+ and Rh3+: ab-initio calculations and prospects for thermophysical and optoelectronic applications. Journal of Molecular Graphics and Modelling, 2020, 101, 107750. | 2.4 | 1 |
| 34 | Magnetic and electrical properties of Ba2Co2Fe12O22/PANI composites prepared by insitu polymerization. Physica B: Condensed Matter, 2020, 597, 412410. | 2.7 | 4 |
| 35 | Effect of Fe doping on optoelectronic properties of CdS nanostructure: Insights from DFT calculations. Physica B: Condensed Matter, 2020, 583, 412056. | 2.7 | 11 |
| 36 | Structural, electronic, optoelectronic and transport properties of LuZnCuAs2 compound: First principle calculations under DFT. Physica B: Condensed Matter, 2020, 596, 412351. | 2.7 | 10 |

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|---|---|---|---|
| 37 | Study of electrical attributes of molybdenum ditelluride (MoTe2) FET using experimental and theoretical evidences. Microelectronic Engineering, 2020, 230, 111365. | 2.4 | 3 |
| 38 | Revealing the optoelectronic properties of Re-based double perovskites using the Tran-Blaha modified Becke-Johnson with density functional theory. Journal of Molecular Modeling, 2020, 26, 158. | 1.8 | 9 |
| 39 | Exploring the potential use of Ca[LiAl3N4]:Eu2+ as phosphor-LED material: Ab-initio calculations. Materials Today Communications, 2020, 25, 101302. | 1.9 | 3 |
| 40 | A first-principles investigation on electronic, optical and thermoelectric properties of $$hbox {La}_{2}hbox {Pd}_{2}hbox {O}_{5}$$ compound. Bulletin of Materials Science, 2020, 43, 1. | 1.7 | 1 |
| 41 | Electronic structure and related optical, thermoelectric and dynamical properties of Lilianite-type Pb7Bi4Se13: Ab-initio and Boltzmann transport theory. Materialia, 2020, 10, 100658. | 2.7 | 11 |
| 42 | Ab-initio study of Cu-based oxychalcogenides: A new class of materials for optoelectronic applications. Journal of Solid State Chemistry, 2020, 284, 121191. | 2.9 | 5 |
| 43 | An effectual enhancement to the electrical conductivity of graphene FET by silver nanoparticles. Diamond and Related Materials, 2020, 106, 107833. | 3.9 | 10 |
| 44 | Nanosized Magnesium doped Copper Chromites Spinel Particles Synthesis and Characterization. ECS Journal of Solid State Science and Technology, 2020, 9, 126005. | 1.8 | 10 |
| 45 | Electronic structure and optical properties of TaNO: An ab initio study. Journal of Molecular Graphics and Modelling, 2019, 92, 296-302. | 2.4 | 15 |
| 46 | Density Functional Theory Investigations of the Optoelectronic Properties of Li2MnGeS4 and Li2CoSnS4. Spin, 2019, 09, 1950015. | 1.3 | 1 |
| 47 | First-Principles Description of the Different Phases in the Li2NH Compound: Electronic Structure and Optical Properties. Journal of the Korean Physical Society, 2019, 74, 1140-1145. | 0.7 | 15 |
| 48 | Gate dependent phonon shift in tungsten disulfide (WS<sub>2</sub>) field effect transistor. Materials Research Express, 2019, 6, 115909. | 1.6 | 11 |
| 49 | DFT study of the electronic and optical properties of ternary chalcogenides AlX<sub>2</sub>Te<sub>4</sub>. Materials Research Express, 2019, 6, 116314. | 1.6 | 33 |
| 50 | A Systematic First-Principles Investigation of Structural, Electronic, Magnetic, and Thermoelectric Properties of Thorium Monopnictides ThPn (Pnâ€‰=â€‰N, P, As): A Comparative Analysis of Theoretical Predictions of LDA, PBEsol, PBE-GGA, WC-GGA, and LDAâ€‰+â€‰U Methods. International Journal of Thermophysics, 2019, 40, 1. | 2.1 | 16 |
| 51 | Tailoring the electrical properties of MoTe2 field effect transistor via chemical doping. Superlattices and Microstructures, 2019, 135, 106247. | 3.1 | 35 |
| 52 | DFT simulations of optoelectronic and elastic features of cubic samarium zirconate (Sm2Zr2O7). Computational Condensed Matter, 2019, 21, e00414. | 2.1 | 3 |
| 53 | Effect of pressure and Hubbard potential on the electronic and magnetic properties of thorium monopnictides ThPn (PnÂ= N, P, As, Sb, Bi) in respect of crystal field splitting, charge transfer and spin flipping of magnetic moments. Computational Condensed Matter, 2019, 21, e00403. | 2.1 | 0 |
| 54 | Insight into the Optoelectronic and Thermoelectric Properties of Mn Doped ZnTe from First Principles Calculation. Crystals, 2019, 9, 247. | 2.2 | 4 |

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|---|---|---|---|
| 55 | Density functional theory within spin-orbit coupling and hubbard correction for investigation of optoelectronic properties of the orthorhombic perovskite LaPdO3. Computational Condensed Matter, 2019, 21, e00396. | 2.1 | 11 |
| 56 | Effect of S and Se replacement on electronic and thermoelectric features of BaCu2GeQ4 (QÂ= S, Se) chalcogenide crystals. Journal of Alloys and Compounds, 2019, 790, 666-674. | 5.5 | 21 |
| 57 | A first-principles theoretical investigation of the structural, electronic and magnetic properties of cubic thorium carbonitrides ThCxN(1-x). Nuclear Engineering and Technology, 2019, 51, 1373-1380. | 2.3 | 6 |
| 58 | A comparative study of structural, electronic and magnetic properties of DyOCl and HoOCl lanthanide oxychlorides: first-principles predictions of DFT, DFT + U and DFT + U + SOC methods. Materials Research Express, 2019, 6, 126129. | 1.6 | 2 |
| 59 | Doping induced effect on optical and band structure properties of Sr2Si5N8 based phosphors: DFT approach. Journal of Alloys and Compounds, 2019, 771, 1072-1079. | 5.5 | 14 |
| 60 | Elastic and optoelectronic properties of CaTa2O6 compounds: Cubic and orthorhombic phases. Journal of Alloys and Compounds, 2019, 785, 232-239. | 5.5 | 31 |
| 61 | Enhanced thermoelectric properties of ASbO3 due to decreased band gap through modified becke johnson potential scheme. Journal of Physics and Chemistry of Solids, 2018, 119, 85-93. | 4.0 | 19 |
| 62 | Electronic structure and thermoelectric properties of PbS1-xTex (x=0, 0.25, 0.50, 0.75, 1.0) alloys: Ab initio study. Superlattices and Microstructures, 2018, 124, 248-256. | 3.1 | 6 |
| 63 | Effects of compressed strain on thermoelectric properties of Cu3SbSe4. Journal of Alloys and Compounds, 2018, 750, 804-810. | 5.5 | 17 |
| 64 | Optoelectronic and Thermoelectric Properties of Bi2OX2 (XÂ=ÂS, Se, Te) for Solar Cells and Thermoelectric Devices. Journal of Electronic Materials, 2018, 47, 2513-2518. | 2.2 | 21 |
| 65 | Electronic and Thermoelectric Properties of Ternary Chalcohalide Semiconductors: First Principles Study. Journal of Electronic Materials, 2018, 47, 1131-1139. | 2.2 | 17 |
| 66 | Optoelectronic Structure and Related Transport Properties of Ag2Sb2O6 and Cd2Sb2O7. Journal of Electronic Materials, 2018, 47, 1481-1489. | 2.2 | 6 |
| 67 | Systematic studies of the structural and optoelectronic characteristics of CaZn<sub>2</sub>X<sub>2</sub>(X = N, P, As, Sb, Bi). Materials Research Express, 2018, 5, 016304. | 1.6 | 19 |
| 68 | Spin Gapless Semiconductorâ€“Nonmagnetic Semiconductor Transitions in Fe-Doped Ti2CoSi: First-Principle Calculations. Applied Sciences (Switzerland), 2018, 8, 2200. | 2.5 | 3 |
| 69 | First-principles calculations of optoelectronic properties of CaO: Eu+2 (SrO: Eu+2) for energy applications. International Journal of Modern Physics B, 2018, 32, 1850333. | 2.0 | 12 |
| 70 | First-principles investigation of the electronic band structures and optical properties of quaternary ABaMQ<sub>4</sub> (A = Rb, Cs; M = P, V; and Q = S) metal chalcogenides. International Journal of Modern Physics B, 2018, 32, 1850337. | 2.0 | 0 |
| 71 | Effect of Coulomb interactions on optoelectronic and magnetic properties of novel A2V2O7 (A= Fe) Tj ETQq1 1 0.784314 rgBT /Overlo | 5.5 | 17 |
| 72 | Specific thermoelectric features of novel CaPd3B4O12 (B = Ti, V) perovskites following DFT calculations. Physica B: Condensed Matter, 2018, 545, 330-336. | 2.7 | 4 |

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|---|---|---|---|
| 73 | Specific features of structural, electronic, optical and elastic properties of the cubic calcium pyroniobate Ca2Nb2O7 crystals. Physica B: Condensed Matter, 2018, 545, 69-75. | 2.7 | 10 |
| 74 | Exploring the optoelectronic properties of Nitrido-magneso-silicates: Ca[Mg3SiN4], Sr[Mg3SiN4], and Eu[Mg3SiN4]. Semiconductor Science and Technology, 2017, 32, 055017. | 2.0 | 2 |
| 75 | Predicted Thermoelectric Properties of the Layered XBi4S7 (XÂ=ÂMn, Fe) Based Materials: First Principles Calculations. Journal of Electronic Materials, 2017, 46, 23-29. | 2.2 | 11 |
| 76 | Polymorph phosphor SrSi2O2N2:Eu2+ optoelectronic properties for highly efficient LED: ab-initio calculations. Materials Today Communications, 2017, 13, 263-268. | 1.9 | 4 |
| 77 | Structural, elastic, optoelectronic and magnetic properties of $$mathbf{CdHo }_mathbf{2}{} mathbf{S}_mathbf{4}$$ CdHo 2 S 4 spinel: a first-principle study. Bulletin of Materials Science, 2017, 40, 1105-1110. | 1.7 | 3 |
| 78 | DFT study of optoelectronic and magnetic properties of iron-containing diamond-like materials Ag 2 FeSiS 4 , Li 2 FeSnS 4 , and Li 2 FeGeS 4. Solid State Sciences, 2017, 72, 71-79. | 3.2 | 5 |
| 79 | Tailoring the electronic structure and optical properties of cadmium-doped zinc oxides nanosheet. Cogent Physics, 2017, 4, 1391734. | 0.7 | 11 |
| 80 | Exploring the thermoelectric and magnetic properties of uranium selenides: Tl2Ag2USe4 and Tl3Cu4USe6. Journal of Magnetism and Magnetic Materials, 2016, 413, 57-64. | 2.3 | 5 |
| 81 | Elastic and optoelectronic properties of novel Ag3AuSe2 and Ag3AuTe2 semiconductors. Materials Science in Semiconductor Processing, 2016, 52, 8-15. | 4.0 | 7 |
| 82 | Optoelectronic structure and related transport properties of BiCuSeO-based oxychalcogenides: First principle calculations. Solid State Sciences, 2016, 58, 86-93. | 3.2 | 26 |
| 83 | DFT combined to Boltzmann transport theory for optoelectronic and thermoelectric properties investigations for monoclinic metallic selenide: Cu5Sn2Se7. Optik, 2016, 127, 5472-5478. | 2.9 | 10 |
| 84 | Engel-Vosko GGA Approach Within DFT Investigations of the Optoelectronic Structure of the Metal Chalcogenide Semiconductor CsAgGa2Se4. Journal of Electronic Materials, 2016, 45, 746-754. | 2.2 | 4 |
| 85 | Interrelationship between structural, optical and transport properties of InP1â^'Bi : DFT approach. Materials Science in Semiconductor Processing, 2016, 41, 45-53. | 4.0 | 12 |
| 86 | Half-metallic ferromagnetism in Be1â^'x V x Te alloys: an Ab-initio study. Indian Journal of Physics, 2015, 89, 1251-1263. | 1.8 | 24 |
| 87 | Electronic structure, chemical bonding and optical properties of Di-2-pyrymidonium dichloride diiodide (C4H5ClIN2O) from first-principles. Materials Science in Semiconductor Processing, 2015, 31, 372-379. | 4.0 | 1 |
| 88 | Theoretical investigation of electronic structure and optical response in relation to the transport properties of Ga1â^'xInxN (xÂ=Â0, 0.25, 0.50, 0.75). Current Applied Physics, 2015, 15, 608-616. | 2.4 | 4 |
| 89 | Theoretical study of the new zintl phases compounds K2ACdSb2 (A=(Sr, Ba)). Physica B: Condensed Matter, 2015, 464, 9-16. | 2.7 | 0 |
| 90 | GGA+U study on phase transition, optoelectronic and magnetic properties of AmO2 with spinâ€“orbit coupling. Journal of Magnetism and Magnetic Materials, 2015, 396, 190-197. | 2.3 | 4 |

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|---|---|---|---|
| 91 | Revealing the optoelectronic and thermoelectric properties of the Zintl quaternary arsenides ACdGeAs2 (A = K, Rb). Materials Research Bulletin, 2015, 70, 847-855. | 5.2 | 39 |
| 92 | Exploring the electronic structure and optical properties of new inorganic luminescent materials Ba(Si,Al)5(O,N)8 compounds for light-emitting diodes devices. Current Applied Physics, 2015, 15, 1160-1167. | 2.4 | 15 |
| 93 | Exploring the electronic structure and optical properties of the quaternary selenide compound, Ba4Ga4SnSe12: For photovoltaic applications. Journal of Solid State Chemistry, 2015, 229, 260-265. | 2.9 | 13 |
| 94 | Electronic structure and optical properties of CdO from bulk to nanosheet: DFT approach. Optical Materials, 2015, 47, 372-378. | 3.6 | 23 |
| 95 | Detailed DFT studies of the electronic structure and optical properties of KBaMSe3 (M = As, Sb). Journal of Alloys and Compounds, 2015, 644, 91-96. | 5.5 | 13 |
| 96 | First principle investigation of electronic structure, chemical bonding and optical properties of tetrabarium gallium trinitride oxide single crystal. Materials Research Bulletin, 2015, 70, 436-441. | 5.2 | 3 |
| 97 | A first principles study of electronic and optical properties of the polar quaternary chalcogenides Î²-A2Hg3Ge2S8(A=K and Rb). Materials Science in Semiconductor Processing, 2015, 34, 250-259. | 4.0 | 15 |
| 98 | Modified Beckeâ€“Johnson (mBJ) exchange potential investigations of the optoelectronic structure of the quaternary diamond-like semiconductors Li2CdGeS4 and Li2CdSnS4. Materials Science in Semiconductor Processing, 2015, 39, 606-613. | 4.0 | 18 |
| 99 | Optoelectronic and Magnetic Properties of Eu<sub>2</sub>Si<sub>5</sub>N<sub>8</sub>: An Ab-initio Study. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 2015, 70, 897-904. | 1.5 | 0 |
| 100 | Coulomb interaction and spin-orbit coupling calculations of thermoelectric properties of the quaternary chalcogenides Tl<sub>2</sub>PbXY<sub>4</sub> (X = Zr, Hf and Y = S, Se). Semiconductor Science and Technology, 2015, 30, 105018. | 2.0 | 12 |
| 101 | DFT and modified Becke Johnson (mBJ) potential investigations of the optoelectronic properties of SnGa4Q7 (QÂ=ÂS, Se) compounds: Transparent materials for large energy conversion. Solid State Sciences, 2015, 48, 244-250. | 3.2 | 12 |
| 102 | First-principles calculations of a half-metallic ferromagnet zinc blende Zn 1âˆ'x V x Te. Journal of Magnetism and Magnetic Materials, 2015, 378, 41-49. | 2.3 | 40 |
| 103 | Thermoelectric and optoelectronic properties of a heterocyclic isoxazolone nucleus compound. Materials Science in Semiconductor Processing, 2015, 30, 197-207. | 4.0 | 4 |
| 104 | Ab initio study of the structural, electronic, elastic and thermal properties of RMn2Ge2 (R = Ca, Nd) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 5 | 5.5 | 8 |
| 105 | Thermoelectric, band structure, chemical bonding and dispersion of optical constants of new metal chalcogenides Ba4CuGa5Q12 (Q=S, Se). Journal of Magnetism and Magnetic Materials, 2014, 362, 204-215. | 2.3 | 4 |
| 106 | Electronic structure, Fermi surface topology and spectroscopic optical properties of LaBaCo2O5.5 compound. Journal of Magnetism and Magnetic Materials, 2014, 363, 133-139. | 2.3 | 5 |
| 107 | The electronic structure, electronic charge density and optical properties of the diamond-like semiconductor Ag2ZnSiS4. Applied Physics A: Materials Science and Processing, 2014, 116, 333-340. | 2.3 | 2 |
| 108 | Electrical transport properties of potassium germanide tungstates (K10Ge18WO4): A theoretical study. Solid State Sciences, 2014, 32, 26-34. | 3.2 | 5 |

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|---|---|---|---|
| 109 | First principle study of the electronic structure, Fermi surface, electronic charge density and optical properties of ThCu5In and ThCu5Sn single crystals. Journal of Magnetism and Magnetic Materials, 2014, 352, 72-80. | 2.3 | 4 |
| 110 | Electronic structure, Fermi surface and optical properties of metallic compound Be8(B48)B2. Journal of Magnetism and Magnetic Materials, 2014, 351, 98-103. | 2.3 | 9 |
| 111 | Transport properties of APdCu(Se<sub>2</sub>)(Se<sub>3</sub>) (A = K and Rb): new quaternary copper palladium polyselenides. RSC Advances, 2014, 4, 20102-20113. | 3.6 | 7 |
| 112 | Optoelectronic behavior of Quaternary Uranium Chalcogenides Rb 2 Pd 3 UM 6 (M = S, Se): A first principle study. Journal of Alloys and Compounds, 2014, 615, 507-513. | 5.5 | 4 |
| 113 | Electronic, optical and thermoelectric properties of Ce3PdIn11 and Ce5Pd2In19: An ab initio study. Intermetallics, 2014, 55, 184-194. | 3.9 | 6 |
| 114 | Theoretical calculations for MUO3 (MÂ=ÂNa; K; Rb): DFTÂ+ÂU study. Journal of Organometallic Chemistry, 2014, 766, 22-33. | 1.8 | 8 |
| 115 | Thermoelectric properties of quaternary Uranium chalcogenides Cs2Pt3US6 and Cs2Pt3USe6. Solid State Sciences, 2014, 34, 56-62. | 3.2 | 2 |
| 116 | Electronic structure, effective mass, and optical dispersion of 2-mercapto-5-methyl-1,3,4-thiadiazole: density functional theory calculations. Materials Science in Semiconductor Processing, 2014, 26, 649-656. | 4.0 | 6 |
| 117 | Linear and nonlinear optical properties of Î±-K2Hg3Ge2S8 and Î±-K2Hg3Sn2S8 compounds. Optical Materials, 2014, 37, 97-103. | 3.6 | 13 |
| 118 | Density of states, optical and thermoelectric properties of perovskite vanadium fluorides Na3VF6. Journal of Magnetism and Magnetic Materials, 2014, 358-359, 16-22. | 2.3 | 6 |
| 119 | First-principles study of the electronic structure, charge density, Fermi surface and optical properties of zintl phases compounds Sr 2 ZnA 2 (A=P, As and Sb). Journal of Magnetism and Magnetic Materials, 2013, 345, 294-303. | 2.3 | 14 |
| 120 | Study of electronic structure, charge density, Fermi energy and optical properties of Cs2KTbCl6 and Cs2KEuCl6. Physica B: Condensed Matter, 2013, 431, 102-108. | 2.7 | 10 |
| 121 | Electronic band structure and specific features of Sm2NiMnO6 compound: DFT calculation. Journal of Magnetism and Magnetic Materials, 2013, 342, 80-86. | 2.3 | 23 |