

# Ghulam Murtaza

## List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/248752/publications.pdf>

Version: 2024-02-01

185  
papers

4,449  
citations

117453

34  
h-index

174990

52  
g-index

187  
all docs

187  
docs citations

187  
times ranked

2968  
citing authors

#	ARTICLE	IF	CITATIONS
1	Hybrid functional calculations of optoelectronic properties of ultra-wide bandgap LiSmO <sub>2</sub> : A first-principle study. Solid State Communications, 2022, 342, 114619.	0.9	4
2	Investigations of $2D Ti_3 C_2$ (MXene) $\text{\AA}$ - $CoCr_2 O_4$ nanocomposite as an efficient electrode material for electrochemical supercapacitors. International Journal of Energy Research, 2022, 46, 6689-6701.	2.2	17
3	First-principles calculations to investigate variation of cationic-ligand $LmAl_2Ge_2$ ( $Lm = Ca, Y, La$ and $Ce$ ). Indian Journal of Physics, 2022, 96, 3151-3159.	0.9	5
4	Effect of layer sliding on the interfacial electronic properties of intercalated silicene/indium selenide van der Waals heterostructure. Communications in Theoretical Physics, 2022, 74, 035701.	1.1	8
5	First-principles study on the electronic band profiles, structural, mechanical and thermoelectric properties of semiconducting $MgSc_2Te_4$ and $MgY_2Te_4$ Spinel. European Physical Journal Plus, 2022, 137, 1.	1.2	5
6	Thermoelectric, structural, electronic, magnetic, and thermodynamic properties of $CaZn_2Ge_2$ compound. European Physical Journal Plus, 2022, 137, 1.	1.2	10
7	Modeling of bulk modulus of $A_2BX_6$ cubic crystals ( $A = K, Cs, Rb, Tl, NH_4$ ; $B =$ tetravalent cation; $X = F, Cl, Br, I$ ). Journal of Materials Science: Materials Chemistry and Physics, 2022, 253, 10784314.	1.8	7
8	Effects of anion-ligands replacement on the Structural, Electronic and Magnetic properties of $ThCo_2X_2$ ( $X = As, Ge$ ). Chinese Journal of Physics, 2022, 77, 956-964.	2.0	8
9	Predicting Lattice Constants of Half-Heusler Alloys Through Deep Neural Network Models Using Symbols of Elements and/or Ionic Radii. Spin, 2022, 12, .	0.6	0
10	A two-step clustering to minimize redundant transmission in wireless sensor network using sleep-awake mechanism. Wireless Networks, 2022, 28, 2077-2104.	2.0	7
11	Engineering of Transition Metal Sulfide Nanostructures as Efficient Electrodes for High-Performance Supercapacitors. ACS Applied Energy Materials, 2022, 5, 6481-6498.	2.5	68
12	Impact of 5d electrons on half metallic ferromagnetism, and thermoelectric properties of $Cs_2Z(Cl/Br)_6$ ( $Z = Os, Ir$ ) for spintronic applications. Materials Chemistry and Physics, 2022, 288, 126414.	2.0	17
13	Influence of the spin-orbit coupling effect on the electronic and thermoelectric properties of $Cs_2MI_6$ ( $M = Zr, Hf$ ) variant perovskites. Materials Research Bulletin, 2021, 134, 111112.	2.7	11
14	An investigation of half-metallic variant perovskites $A_2NbCl_6$ ( $A = K, Rb$ ) for spintronic based applications. Journal of Solid State Chemistry, 2021, 293, 121823.	1.4	14
15	Structural, electronic and optoelectronic properties of $AB_5 C_8$ ( $A = Cu/Ag$ ; $B = In$ and $C = S, Se$ and $Te$ ) compounds. International Journal of Energy Research, 2021, 45, 4014-4025.	2.2	4
16	Optoelectronic and transport properties of $Rb/Cs_2 Te_6$ defective perovskites for green energy applications. International Journal of Energy Research, 2021, 45, 8448-8455.	2.2	16
17	Study of Optoelectronic and Thermoelectric Characteristics of Cesium Based Halides $CsYbX_3$ ( $X = Br, Cl$ ) for Clean Energy Harvesting. ECS Journal of Solid State Science and Technology, 2021, 10, 015002.	0.9	5
18	Pressure-dependent elastomeric stability and thermoelectric properties of $MYbF_3$ ( $M = Rb, Cs$ ) materials for renewable energy. International Journal of Energy Research, 2021, 45, 8711-8723.	2.2	48

#	ARTICLE	IF	CITATIONS
19	Prediction of novel $X_2ZnZ_4$ ( $X = Sc, Y; Z = S, Se$ ) spinels materials for renewable energy applications. International Journal of Energy Research, 2021, 45, 8307-8315.	2.2	5
20	Anionic variations for $BaMg_2X_2$ ( $X = N$ to $Bi$ ) compounds by density functional theory. European Physical Journal Plus, 2021, 136, 1.	1.2	13
21	First principles calculations of structural, electronic, optical, and thermoelectric properties of ternary $XY_2Z_4$ metal sulfides ( $Sc_2CdS_4$ and $Y_2CdS_4$ ) compounds. International Journal of Energy Research, 2021, 45, 13657-13667.	2.2	9
22	Electronic and optical properties of vacancy ordered double perovskites $A_2BX_6$ ( $A = Rb, Cs; B = Sn, Pd, Pt$ ). Journal of Energy Research, 2021, 45, 13668-13678.	1.6	78
23	First principle study of structural, electronic, optical and mechanical properties of cubic fluoro-perovskites: ( $CdXF_3$ , $X = Y, Bi$ ). European Physical Journal Plus, 2021, 136, 1.	1.2	36
24	Machine learning-based offline signature verification systems: A systematic review. Signal Processing: Image Communication, 2021, 93, 116139.	1.8	23
25	A hybridization strategy using equal and unequal clustering schemes to mitigate idle listening for lifetime maximization of wireless sensor network. Wireless Networks, 2021, 27, 2641-2670.	2.0	3
26	$Co_2YZ$ ( $Y = Cr, Nb, Ta, V$ and $Z = Al, Ga$ ) Heusler alloys under the effect of pressure and strain. Journal of Molecular Graphics and Modelling, 2021, 104, 107841.	1.3	46
27	Spin-based transport properties of $Cs_2WX_6$ ( $X = Cl, Br$ ) ferromagnets for spin-injected thermoelectric current. European Physical Journal Plus, 2021, 136, 1.	1.2	12
28	Defective perovskites $Cs_2SeCl_6$ and $Cs_2TeCl_6$ as novel high temperature potential thermoelectric materials. Materials Science in Semiconductor Processing, 2021, 127, 105728.	1.9	33
29	Insights into the structural, electronic and optical properties of $MgA_2B_4$ ( $A = Sc, Y; B = S, Se$ ) spinel compounds: Direct energy band gap materials. Materials Science in Semiconductor Processing, 2021, 127, 105736.	1.9	6
30	Systematic investigation of magnetic, optical and transport properties of $RTX$ ( $R =$ Rare earth, $T = 3d/4d$ ). Journal of Energy Research, 2021, 45, 2150212.	1.0	0
31	Study of optical and thermoelectric properties of $ZYbI_3$ ( $Z = Rb, Cs$ ) for solar cells and renewable energy; Modelling by density functional theory. Journal of Physics and Chemistry of Solids, 2021, 155, 110117.	1.9	18
32	Study of optoelectronic and thermoelectric properties of double perovskites for renewable energy. Physica Scripta, 2021, 96, 125828.	1.2	12
33	First principle study of half metallic ferromagnetism and transport properties of spinel $ZnFe_2(S/Se)_4$ for spintronic. Physica Scripta, 2021, 96, 125816.	1.2	10
34	Synthesis and characterisation of nanosized spinel particles of nickel-doped iron chromite. Philosophical Magazine Letters, 2021, 101, 464-473.	0.5	7
35	First principle study of optoelectronic and thermoelectric properties of magnesium based $MgX_2O_4$ ( $X =$ ). Journal of Energy Research, 2021, 45, 13679-13684.	1.4	14
36	Appealing perspectives of structural, electronic, mechanical, and thermoelectric properties of $Tl_2(Se)$ . Journal of Energy Research, 2021, 45, 110258.	1.9	34

#	ARTICLE	IF	CITATIONS
37	Different physical properties of alkali pnictogen compounds using density functional theory. International Journal of Energy Research, 2021, 45, 7703-7718.	2.2	10
38	Computational investigation of structural, magnetic, elastic, and electronic properties of Half-Heusler ScVX (X=Si, Ge, Sn, and Pb) compounds. European Physical Journal Plus, 2021, 136, 1.	1.2	10
39	First-principles calculations for optoelectronic properties of AlSb and GaSb under influence of spin-orbit interaction effect. Indian Journal of Physics, 2020, 94, 477-484.	0.9	14
40	Deep learning-based breast cancer classification through medical imaging modalities: state of the art and research challenges. Artificial Intelligence Review, 2020, 53, 1655-1720.	9.7	161
41	Breast Cancer Multi-classification through Deep Neural Network and Hierarchical Classification Approach. Multimedia Tools and Applications, 2020, 79, 15481-15511.	2.6	40
42	DFT Investigations of Structural, Magnetic, Electronic, and Optical Properties of CsEuCl <sub>3</sub> . Journal of Superconductivity and Novel Magnetism, 2020, 33, 1045-1051.	0.8	15
43	A theoretical study of the structural, thermoelectric, and spin-orbit coupling influenced optoelectronic properties of CsTmCl <sub>3</sub> halide perovskite. International Journal of Quantum Chemistry, 2020, 120, e26141.	1.0	31
44	Electronic and optical properties of Sr <sub>3</sub> X <sub>2</sub> (X=N, P, As, Sb and Bi) compounds: first principles study. Philosophical Magazine, 2020, 100, 768-781.	0.7	6
45	Pressure induced physical variations in the lead free fluoropervoskites XYF <sub>3</sub> (X=K, Rb, Ag; Y=Zn, Sr, Tl) compounds: A first principles study. Journal of Solid State Chemistry, 2020, 292, 121589.	1.7	15
46	Anion replacement effect on BaCd <sub>2</sub> X <sub>2</sub> (X = P, As, Sb, Bi) compounds: A first principles study. Journal of Solid State Chemistry, 2020, 292, 121589.	1.4	8
47	Anion-cation replacement effect in lead free tin based variant perovskites. Physica B: Condensed Matter, 2020, 595, 412345.	1.3	14
48	Smartphone Motion Sensor-Based Complex Human Activity Identification Using Deep Stacked Autoencoder Algorithm for Enhanced Smart Healthcare System. Sensors, 2020, 20, 6300.	2.1	20
49	Structural, electronic, optoelectronic and transport properties of LuZnCuAs <sub>2</sub> compound: First principle calculations under DFT. Physica B: Condensed Matter, 2020, 596, 412351.	1.3	10
50	First Principle Study of Structural, Electronic, Elastic, and Magnetic Properties of Half-Heusler Compounds ScTiX (X=Si, Ge, Pb, In, Sb, and Tl). Journal of Superconductivity and Novel Magnetism, 2020, 33, 3915-3922.	0.8	19
51	Modeling of structural, elastic, mechanical, acoustical, electronic and thermodynamic properties of XPdF <sub>3</sub> (X = Rb, Tl) perovskites through density functional theory. Physica Scripta, 2020, 95, 075705.	1.2	24
52	Theoretical investigation of the structural stabilities, optoelectronic and thermoelectric properties of ternary alloys NaInY <sub>2</sub> (Y = S, Se, Te) through modified Becke-Johnson exchange potential. International Journal of Modern Physics B, 2020, 34, 2050133.	1.0	7
53	Ab initio study for the structural, electronic, magnetic, optical, and thermoelectric properties of K <sub>2</sub> OsX <sub>6</sub> (X = Cl, Br) compounds. International Journal of Energy Research, 2020, 44, 9035-9049.	2.2	36
54	Ensembled deep convolution neural network-based breast cancer classification with misclassification reduction algorithms. Multimedia Tools and Applications, 2020, 79, 18447-18479.	2.6	19

#	ARTICLE	IF	CITATIONS
55	Exploring ferromagnetic half-metallic nature of Cs <sub>2</sub> NpBr <sub>6</sub> via spin polarized density functional theory*. Chinese Physics B, 2020, 29, 066102.	0.7	15
56	Insight into pressure tunable structural, electronic and optical properties of "Equation missing" <!-- No EquationSource Format="TEX", only image --> via DFT calculations. European Physical Journal Plus, 2020, 135, 1.	1.2	32
57	<scp>Magneto-electronic</scp> properties of ferromagnetic compounds <scp>Rb<sub>2</sub>TaZ<sub>6</sub></scp> (Z = Cl, Br) for possible spintronic applications. International Journal of Quantum Chemistry, 2020, 120, e26357.	1.0	9
58	The significance of anti-fluorite <scp>Cs<sub>2</sub>Nbl<sub>6</sub></scp> via its structural, electronic, magnetic, optical and thermoelectric properties. International Journal of Energy Research, 2020, 44, 10179-10191.	2.2	25
59	Study of anion replacement effect on SrCd <sub>2</sub> X <sub>2</sub> (X = P, As, Sb, Bi) compounds by FPLAPW+lo. Materials Science in Semiconductor Processing, 2020, 119, 105290.	1.9	8
60	Scalable and Universal Route for the Deposition of Binary, Ternary, and Quaternary Metal Sulfide Materials from Molecular Precursors. ACS Applied Energy Materials, 2020, 3, 1952-1961.	2.5	30
61	Heterogeneous Energy and Traffic Aware Sleep-Awake Cluster-Based Routing Protocol for Wireless Sensor Network. IEEE Access, 2020, 8, 12232-12252.	2.6	51
62	Probing the electronic structure and magnetism in Ni doped ZnTe: A DFT modeling and experiment. Journal of Alloys and Compounds, 2020, 834, 155176.	2.8	15
63	Theoretical investigations of optoelectronic and thermoelectric properties of the XIn <sub>2</sub> O <sub>4</sub> (X = Mg, Zn, Tl) compounds. Journal of Applied Physics, 2020, 122, 074301.	1.9	22
64	First-principles calculations of electronic and magnetic properties of XMn <sub>2</sub> Y <sub>2</sub> (X = Ca, Sr; Y = Sb, Bi) compounds. International Journal of Modern Physics B, 2019, 33, 1950199.	1.0	24
65	Comprehensive study of the physical properties of Ba <sub>3</sub> Pn <sub>2</sub> (Pn=N, P, As, Sb and Tl) compounds. Journal of Applied Physics, 2019, 125, 074301.	0.8	2
66	DFT prediction of the structural, electronic, thermoelectric and optical properties of ternary pnictides MgBe <sub>2</sub> X <sub>2</sub> (X = N, P, As, Sb, Bi): A novel analysis of beryllium with 2A- and 5B-Elements of the structure type CaAl <sub>2</sub> Si <sub>2</sub> . Solid State Communications, 2019, 300, 113667.	0.9	13
67	First principle study of structural, electronic, optical, and transport properties of ternary compounds NaGaX <sub>2</sub> (X = S, Se, and Te) in tetragonal chalcopyrite phase. Optical and Quantum Electronics, 2019, 51, 1.	1.5	20
68	Synthetic 2-D lead tin sulfide nanosheets with tuneable optoelectronic properties from a potentially scalable reaction pathway. Chemical Science, 2019, 10, 1035-1045.	3.7	16
69	Predicting Cyberbullying on Social Media in the Big Data Era Using Machine Learning Algorithms: Review of Literature and Open Challenges. IEEE Access, 2019, 7, 70701-70718.	2.6	87
70	Electronic and magnetic properties of alkali metal chlorides A <sub>2</sub> MCl <sub>6</sub> (A = K, Tl) compounds. Journal of Applied Physics, 2019, 33, 1950072.	1.0	14
71	First principles investigation of Be <sub>3</sub> X <sub>2</sub> (X = N, P, As) and their alloys for solar cell applications. Journal of Alloys and Compounds, 2019, 795, 385-390.	2.8	5
72	First principles calculations for structural, elastic, mechanical, electronic and optical properties of CsYbCl <sub>3</sub> . Materials Research Express, 2019, 6, 065905.	0.8	23

#	ARTICLE	IF	CITATIONS
73	Investigation of the structural, electrical, optical and magnetic properties of $\text{XMg}_4\text{Mn}_6\text{O}_{15}$ ( $X = \text{K, Rb, and Cs}$ ) compounds. Materials Research Express, 2019, 6, 066102.	0.8	11
74	Breast cancer classification using digital biopsy histopathology images through transfer learning. Journal of Physics: Conference Series, 2019, 1339, 012035.	0.3	6
75	Layer-sliding-mediated controlled tuning of physical properties of intercalated silicene/hBN heterostructure. Materials Research Express, 2019, 6, 035005.	0.8	6
76	Effects of anion replacement on the physical properties of $\text{CaCd}_2\text{X}_2$ ( $X = \text{P, As, Sb, Bi}$ ). Journal of Physics and Chemistry of Solids, 2019, 127, 81-87.	1.9	10
77	First principle study of electronic, mechanical, optical and thermoelectric properties of $\text{CsMO}_3$ ( $M = \text{N, P, As, Sb, Bi}$ ). Journal of Physics and Chemistry of Solids, 2018, 119, 157-165.	1.3	45
78	Electronic band profiles and optical response of $\text{Cd}_3\text{Y}_2$ ( $Y = \text{N, P and As}$ ) compounds. Journal of Physics and Chemistry of Solids, 2018, 119, 157-165.	1.9	2
79	Effect of Varying Pnictogen Elements ( $\text{Pn} = \text{N, P, As, Sb, Bi}$ ) on the Optoelectronic Properties of $\text{SrZn}_2\text{Pn}_2$ . Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 2018, 73, 285-293.	0.7	25
80	Synthesis, characterisation and photocatalytic performance of ZnS coupled $\text{Ag}_2\text{S}$ nanoparticles: A remediation model for environmental pollutants. Arabian Journal of Chemistry, 2018, 11, 827-837.	2.3	28
81	The effect of replacing pnictogen elements on the physical properties $\text{SrMg}_2\text{X}_2$ ( $X = \text{N, P, As, Sb, Bi}$ ) Zintl compounds. Chinese Physics B, 2018, 27, 047102.	0.7	22
82	Impact of anion replacement on the optoelectronic and thermoelectric properties of $\text{CaMg}_2\text{X}_2$ , $X = (\text{N, P, As, Sb, Bi})$ . Journal of Physics and Chemistry of Solids, 2018, 119, 157-165.	1.3	21
83	The Effects of Ru and Rh Substitutions on the Magneto-electronic and Optical Properties of the $\text{TbNi}_5$ Intermetallic Compound: An Ab Initio Investigation. Journal of Superconductivity and Novel Magnetism, 2018, 31, 547-559.	0.8	2
84	Ab Initio Investigation of the Structural, Electronic and Optical Properties of the $\text{Li}_2\text{In}_2\text{XY}_6$ ( $X = \text{Si, Ge}$ ). Journal of Physics and Chemistry of Solids, 2018, 119, 157-165.	1.0	50
85	Systematic studies of the structural and optoelectronic characteristics of $\text{CaZn}_2\text{X}_2$ ( $X = \text{N, P, As, Sb, Bi}$ ). Materials Research Express, 2018, 5, 016304.	0.8	19
86	Electronic, optical and thermoelectric properties of $\text{SnGa}_2\text{GeX}_6$ ( $X = \text{S, Se}$ ) compounds. Journal of Alloys and Compounds, 2018, 737, 637-645.	2.8	7
87	Ab-initio prediction of structural, electronic and magnetic properties of Hexafluoromanganate(IV) complexes. International Journal of Modern Physics B, 2018, 32, 1850270.	1.0	9
88	Structural investigations of $\text{SnS}_{1-x}\text{Se}_x$ solid solution synthesized from chalcogeno-carboxylate complexes of organo-tin by colloidal and solvent-less routes. Dalton Transactions, 2018, 47, 10025-10034.	1.6	36
89	Ab-initio study of Li based chalcopyrite compounds $\text{LiGaX}_2$ ( $X = \text{S, Se, Te}$ ) in tetragonal symmetry: A class of future materials for optoelectronic applications. Current Applied Physics, 2018, 18, 1113-1121.	1.1	20
90	Structural, Optoelectronic and Thermoelectric Properties of Ternary $\text{CaBe}_2\text{X}_2$ ( $X = \text{N, P, As, Sb, Bi}$ ) Compounds. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 2018, 73, 965-973.	0.7	18

#	ARTICLE	IF	CITATIONS
91	Anion-Cation Replacement Effect on the Structural and Optoelectronic Properties of the $\text{LiMX}_2$ ( $M = \text{Al, Ga, In}$ ; $X = \text{S, Se, Te}$ ) Compounds: A First Principles Study. <i>Zeitschrift für Naturforschung - Section A Journal of Physical Sciences</i> , 2018, 73, 645-655.		7
92	Chemical vapour deposition of chromium-doped tungsten disulphide thin films on glass and steel substrates from molecular precursors. <i>Journal of Materials Chemistry C</i> , 2018, 6, 9537-9544.	2.7	8
93	Photocatalytic removal of carcinogenic reactive red S3B dye by using ZnO and Cu doped ZnO nanoparticles synthesized by polyol method: A kinetic study. <i>Solar Energy</i> , 2018, 173, 875-881.	2.9	30
94	Synthesis of chalcopyrite-type and thiospinel minerals/materials by low temperature melts of xanthates. <i>Dalton Transactions</i> , 2018, 47, 8870-8873.	1.6	31
95	GGA and GGA + U Study of Rare Earth-Based Perovskites in Cubic Phase. <i>Journal of Superconductivity and Novel Magnetism</i> , 2017, 30, 1389-1396.	0.8	26
96	Formation and Characterization of Model Iron Sulfide Scales with Disulfides and Thiols on Steel Pipeline Materials by an Aerosol-Assisted Chemical Vapor Method. <i>Energy &amp; Fuels</i> , 2017, 31, 2496-2500.	2.5	0
97	Structural, electronic, optical and thermoelectric properties of $\text{Mg}_3\text{X}_2$ ( $X = \text{N, P, As, Sb, Bi}$ ) compounds. <i>Materials Research Bulletin</i> , 2017, 91, 22-30.	2.7	28
98	Exploring the versatility of liquid phase exfoliation: producing 2D nanosheets from talcum powder, cat litter and beach sand. <i>2D Materials</i> , 2017, 4, 025054.	2.0	39
99	Ab Initio Investigations of Structural, Elastic, Mechanical, Electronic, Magnetic, and Optical Properties of Half-Heusler Compounds $\text{RhCrZ}$ ( $Z = \text{Si, Ge}$ ). <i>Journal of Superconductivity and Novel Magnetism</i> , 2017, 30, 2481-2488.	0.8	49
100	Band structure features, chemical bonding and optical properties of $\text{Zn}_3\text{X}_2$ ( $X = \text{N, P, As}$ ) compounds. <i>Journal of Alloys and Compounds</i> , 2017, 728, 1226-1234.	2.8	16
101	First principles investigations of electronics, magnetic, and thermoelectric properties of rare earth based $\text{PrYO}_3$ ( $Y = \text{Cr, V}$ ) perovskites. <i>Current Applied Physics</i> , 2017, 17, 1539-1546.	1.1	93
102	Ab initio study of the electronic and optical properties of $\text{Ag}_3\text{AuS}_2$ polymorphs. <i>Materials Research Express</i> , 2017, 4, 085907.	0.8	2
103	Engel-Vosko GGA calculations of the structural, electronic and optical properties of $\text{LiYO}_2$ . <i>Physica B: Condensed Matter</i> , 2017, 521, 62-68.	1.3	10
104	First principles study of the structural and optoelectronic properties of the $\text{A}_2\text{InSbO}_6$ ( $A = \text{Ca, Sr, Ba}$ ) compounds. <i>Optik</i> , 2017, 130, 517-524.	1.4	44
105	Tailoring the electronic structure and optical properties of cadmium-doped zinc oxides nanosheet. <i>Cogent Physics</i> , 2017, 4, 1391734.	0.7	11
106	Structural, elastic, electronic and magnetic properties of $\text{Ba}_2\text{XOsO}_6$ ( $X = \text{Li, Na, Ca}$ ) double perovskites. <i>Indian Journal of Physics</i> , 2016, 90, 1225-1231.	0.9	5
107	First Principles Investigation of the Elastic, Optoelectronic and Thermal Properties of $\text{XRuSb}$ : ( $X = \text{V, Tj}$ ) <i>ETQq1 1 0.784314 rgBT /Over</i> 2016, 45, 3479-3490.	1.0	46
108	Electronic and Optical Properties of $\text{Ca}_3\text{MN}$ ( $M = \text{Ge, Sn, Pb, P, As, Sb and Bi}$ ) Antiperovskite Compounds. <i>Journal of Electronic Materials</i> , 2016, 45, 4188-4196.	1.0	18



#	ARTICLE	IF	CITATIONS
109	Structural, elastic, electronic and optical properties of bi-alkali antimonides. Bulletin of Materials Science, 2016, 39, 1581-1591.	0.8	21
110	First-principles study of the double perovskites Sr <sub>2</sub> XO <sub>6</sub> (X = Li, Na, Ca) for spintronics applications. Bulletin of Materials Science, 2016, 39, 1419-1425.	0.8	53
111	Photo-sensitization of ZnS nanoparticles with renowned ruthenium dyes N3, N719 and Z907 for application in solid state dye sensitized solar cells: A comparative study. Journal of Photochemistry and Photobiology B: Biology, 2016, 162, 583-591.	1.7	42
112	Computational study of Cu <sub>2</sub> ZnSn(X <sub>1-x</sub> Tex) <sub>4</sub> (X = S, Se) for optoelectronic applications. International Journal of Modern Physics B, 2016, 30, 1650137.	1.0	4
113	Structural, optoelectronic, and thermoelectric properties of AZn <sub>13</sub> (A=Na, K, Ca, Sr, Ba) compounds. International Journal of Modern Physics B, 2016, 30, 1650221.	1.0	3
114	Investigating the Structural, Thermal, and Electronic Properties of the Zircon-Type ZrSiO <sub>4</sub> , ZrGeO <sub>4</sub> and HfSiO <sub>4</sub> Compounds. Journal of Electronic Materials, 2016, 45, 5811-5821.	1.0	11
115	Structural and Optoelectronic Properties of X <sub>3</sub> ZN (X=Ca, Sr, Ba; Z=As, Sb, Bi) Anti-Perovskite Compounds. Journal of Electronic Materials, 2016, 45, 3059-3068.	1.0	23
116	Direct band gap nature and optical response of BexMgyZn <sub>1-x-y</sub> Se. Modern Physics Letters B, 2016, 30, 1650007.	1.0	2
117	Structural, electronic, elastic, thermoelectric and thermodynamic properties of the NbMSb half heusler (M=Fe, Ru, Os) compounds with first principle calculations. Superlattices and Microstructures, 2016, 93, 171-185.	1.4	31
118	First-principles Investigation of Half-metallicity and Ferrimagnet Properties of Co <sub>2</sub> ScZ (Z = As, Sb, and) Tj ETQq0 0 0 rgBT /Overlock 10 T	0.8	8
119	Electronic, optical and thermoelectric properties of XNMg <sub>3</sub> (X=P, As, Sb, Bi) compounds. Materials Science in Semiconductor Processing, 2016, 43, 69-74.	1.9	13
120	Structural, Magnetic, and Optoelectronic Properties of TbNi <sub>5</sub> , TbNi <sub>3</sub> Ti <sub>2</sub> and TbNi <sub>3</sub> V <sub>2</sub> Compounds. Journal of Superconductivity and Novel Magnetism, 2016, 29, 1255-1266.	0.8	1
121	Half-metallicity and optoelectronic properties of V-doped zincblende ZnS and CdS alloys. International Journal of Modern Physics B, 2016, 30, 1650034.	1.0	15
122	Electronic, bonding, linear and non-linear optical properties of novel Li <sub>2</sub> Ga <sub>2</sub> Ge <sub>6</sub> compound. Journal of Alloys and Compounds, 2016, 674, 109-115.	2.8	9
123	The study of electronic, elastic, magnetic and optical response of Zn <sub>1-x</sub> Ti <sub>x</sub> Y (Y = S, Se) through mBJ potential. Current Applied Physics, 2016, 16, 549-561.	1.1	27
124	First principles study of structural, optoelectronic and thermoelectric properties of Cu <sub>2</sub> CdSnX <sub>4</sub> (X =) Tj ETQq0 0 0 rgBT /Overlock 10 T	2.7	22
125	First principle study of vanadium doped ZnS: Structural, electronic, elastic, magnetic and optical properties using mBJ approximation. Current Applied Physics, 2016, 16, 361-370.	1.1	36
126	Elastic and electro-optical properties of XYZ (X=Li, Na and K; Y=Mg; Z=N, P, As, Sb and Bi) compounds. Indian Journal of Physics, 2016, 90, 639-647.	0.9	22





#	ARTICLE	IF	CITATIONS
145	Magnetic ordering and electronic structure of the ternary iron arsenide BaFe <sub>2</sub> As <sub>2</sub> . International Journal of Modern Physics B, 2015, 29, 1550182.	1.0	0
146	Optoelectronic properties of XIn <sub>2</sub> S <sub>4</sub> (X = Cd, Mg) thiospinels through highly accurate all-electron FP-LAPW method coupled with modified approximations. Journal of Alloys and Compounds, 2015, 625, 182-187.	2.8	23
147	Structural phase transition and opto-electronic properties of NaZnAs. Journal of Alloys and Compounds, 2015, 622, 812-818.	2.8	1
148	Structural, elastic, electronic, magnetic and optical properties of RbSrX (X = C, Si, Ge) half-Heusler compounds. Journal of Magnetism and Magnetic Materials, 2015, 377, 204-210.	1.0	71
149	First principles study of structural, optical, and electronic properties of zinc mercury chalcogenides. Materials Science in Semiconductor Processing, 2015, 30, 462-468.	1.9	33
150	Spin-polarized structural, elastic, electronic and magnetic properties of half-metallic ferromagnetism in V-doped ZnSe. Journal of Magnetism and Magnetic Materials, 2015, 374, 50-60.	1.0	29
151	Structural, elastic, thermal and electronic properties of M <sub>2</sub> X (M = Sr, Ba and X = Si, Ge, Sn) compounds in anti-fluorite structure: first principle calculations. Indian Journal of Physics, 2015, 89, 369-375.	0.9	10
152	Ab Initio Study of the Mechanical, Thermal and Optoelectronic Properties of the Cubic CsBaF <sub>3</sub> . Acta Physica Polonica A, 2015, 128, 34-42.	0.2	35
153	Investigations of the half-metallic behavior and the magnetic and thermodynamic properties of half-Heusler CoMnTe and RuMnTe compounds: A first-principles study. Chinese Physics B, 2014, 23, 087103.	0.7	28
154	Structural, chemical bonding and optoelectronic properties of Mg doped zinc chalcogenides: A first principles study. Materials Science in Semiconductor Processing, 2014, 26, 681-689.	1.9	32
155	INSULATOR TO METAL TRANSITION AND OPTICAL RESPONSE OF CsCl UNDER PRESSURE. International Journal of Modern Physics B, 2014, 28, 1450047.	1.0	5
156	Structural, electronic, optical and thermodynamic properties of cubic REGa <sub>3</sub> (RE=Sc or Lu) compounds: Ab initio study. Journal of Alloys and Compounds, 2014, 597, 36-44.	2.8	57
157	First principle study of MF <sub>2</sub> (M=Mg, Ca, Sr, Ba, Ra) compounds. Computational Materials Science, 2014, 81, 575-581.	1.4	10
158	Towards from indirect to direct band gap and optical properties of XYP <sub>2</sub> (X=Zn, Cd; Y=Si, Ge, Sn). Physica B: Condensed Matter, 2014, 441, 94-99.	1.3	14
159	Phase transition, electronic and optical properties of mercury chalcogenides under pressure. Phase Transitions, 2014, 87, 571-581.	0.6	23
160	Electronic, optical and bonding properties of MgYZ <sub>2</sub> (Y=Si, Ge; Z=N, P) chalcopyrites from first principles. Materials Science in Semiconductor Processing, 2014, 26, 79-86.	1.9	34
161	Shift of band gap from indirect to direct and optical response of CaO by doping S, Se, Te. Computational Materials Science, 2014, 91, 43-49.	1.4	22
162	Phase transition, electronic and optical properties of III-Sb compounds under pressure. Phase Transitions, 2014, 87, 893-906.	0.6	8

#	ARTICLE	IF	CITATIONS
163	Structural, electronic and optical properties of AgXY <sub>2</sub> (X = Al, Ga, In and Y = S, Se, Te). Journal of Alloys and Compounds, 2014, 617, 575-583.	2.8	37
164	Structural, electronic, and optical properties of orthorhombic and triclinic BiNbO <sub>4</sub> determined via DFT calculations. Journal of Materials Science, 2014, 49, 7809-7818.	1.7	12
165	Structural phase transition, mechanical and optoelectronic properties of the tetragonal NaZnP: Ab-initio study. Computational Materials Science, 2014, 84, 396-403.	1.4	14
166	The effects of 5f localization on the electronic and magnetic properties of the hexagonal U <sub>3</sub> ZrSb <sub>5</sub> . Journal of Alloys and Compounds, 2014, 586, 529-535.	2.8	4
167	Ab initio study of the structural and optoelectronic properties of the half-Heusler CoCrZ (Z = Al, Ga). Canadian Journal of Physics, 2014, 92, 1105-1112.	0.4	60
168	Structural, elastic, electronic and chemical bonding properties of AB (A=Sc,Y,La;B=N,P,As,Sb,Bi) from first principles. Computational Materials Science, 2013, 79, 239-246.	1.4	32
169	Electronic Band Structure and Optical Response of Spinel SnX <sub>2</sub> O <sub>4</sub> (X = Mg, Zn) through Modified Becke-Johnson Potential. Chinese Physics Letters, 2013, 30, 047401.	1.3	13
170	Elastic, optoelectronic, and thermal properties of cubic CSi <sub>2</sub> N <sub>4</sub> : an ab initio study. Journal of Materials Science, 2013, 48, 8235-8243.	1.7	24
171	Electronic and Optical Properties of Spinel GeMg <sub>2</sub> O <sub>4</sub> and GeCd <sub>2</sub> O <sub>4</sub> . Chinese Physics Letters, 2013, 30, 127401.	1.3	4
172	Elastic and optoelectronic properties of RbMF <sub>3</sub> (M=Zn, Cd, Hg): A mBJ density functional calculation. Physica B: Condensed Matter, 2013, 410, 131-136.	1.3	41
173	SHIFT OF BAND GAP FROM DIRECT TO INDIRECT AND OPTICAL RESPONSE OF LiF UNDER PRESSURE. Modern Physics Letters B, 2013, 27, 1350061.	1.0	16
174	ELECTRONIC BAND STRUCTURE, OPTICAL, THERMAL AND BONDING PROPERTIES OF X <sub>2</sub> Mg <sub>2</sub> O <sub>4</sub> (X = Si, Ge) SPINEL COMPOUNDS. International Journal of Modern Physics B, 2013, 27, 1350082.	1.0	9
175	Electronic Band Profile and Optical Response of Spinel MgIn <sub>2</sub> O <sub>4</sub> through Modified Becke-Johnson Potential. Chinese Physics Letters, 2013, 30, 067401.	1.3	8
176	STRUCTURAL, ELASTIC, ELECTRONIC, CHEMICAL BONDING AND OPTICAL PROPERTIES OF M <sub>2</sub> Se (M = Li, Na,) Tj ETQq0 Q0 rgBT /Overlock 10 Physics B, 2013, 27, 1350170.	1.0	8
177	Physical Properties of CsSnM <sub>3</sub> (M = Cl, Br, I): A First Principle Study. Acta Physica Polonica A, 2013, 124, 102-107.	0.2	72
178	Structural, electronic and optical properties of Ca <sub>x</sub> Cd <sub>1-x</sub> O and its conversion from semimetal to wide bandgap semiconductor. Computational Materials Science, 2012, 58, 71-76.	1.4	32
179	Shift of indirect to direct bandgap and optical response of LaAlO <sub>3</sub> under pressure. Journal of Applied Physics, 2012, 111, .	1.1	48
180	Structural and Optoelectronic Properties of Cubic CsPbF <sub>3</sub> for Novel Applications. Chinese Physics Letters, 2011, 28, 117803.	1.3	45

#	ARTICLE	IF	CITATIONS
181	First principle study of cubic perovskites: AgTF <sub>3</sub> (T=Mg, Zn). Physica B: Condensed Matter, 2011, 406, 4584-4589.	1.3	45
182	Linear and nonlinear optical response of Mg <sub>x</sub> Zn <sub>1-x</sub> O: A density functional study. Physica B: Condensed Matter, 2011, 406, 2632-2636.	1.3	25
183	First principle study of the structural and optoelectronic properties of cubic perovskites CsPbM <sub>3</sub> (M=Cl, Br, I). Physica B: Condensed Matter, 2011, 406, 3222-3229.	1.3	263
184	Investigation of structural and optoelectronic properties of BaThO <sub>3</sub> . Optical Materials, 2011, 33, 553-557.	1.7	124
185	Bandgap engineering of Cd <sub>1-x</sub> Sr <sub>x</sub> O. Physica B: Condensed Matter, 2011, 406, 2509-2514.	1.3	33