Ali Hussain Reshak

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/2120349/publications.pdf

Version: 2024-02-01

459 papers	12,407 citations	41258 49 h-index	54797 84 g-index
474 all docs	474 docs citations	474 times ranked	8318 citing authors

#	Article	IF	Citations
1	Macroscopic Polarization Enhancement Promoting Photoâ€•and Piezoelectricâ€Induced Charge Separation and Molecular Oxygen Activation. Angewandte Chemie - International Edition, 2017, 56, 11860-11864.	7.2	850
2	Chlorine intercalation in graphitic carbon nitride for efficient photocatalysis. Applied Catalysis B: Environmental, 2017, 203, 465-474.	10.8	328
3	Elastic, electronic and optical properties of ZnS, ZnSe and ZnTe under pressure. Computational Materials Science, 2006, 38, 29-38.	1.4	278
4	Photoelectrical properties and the electronic structure of Tl1â^'xIn1â^'xSnxSe2 (x = 0, 0.1, 0.2, 0.25) single crystalline alloys. Physical Chemistry Chemical Physics, 2013, 15, 6965.	1.3	167
5	Dispersion of linear and nonlinear optical susceptibilities and the hyperpolarizability of 3-methyl-4-phenyl-5-(2-pyridyl)-1,2,4-triazole. Physical Chemistry Chemical Physics, 2011, 13, 2945-2952.	1.3	155
6	Ab initio study of TaON, an active photocatalyst under visible light irradiation. Physical Chemistry Chemical Physics, 2014, 16, 10558.	1.3	152
7	Linear, non-linear optical susceptibilities and the hyperpolarizability of the mixed crystals Ag0.5Pb1.75Ge(S1â^'xSex)4: experiment and theory. Physical Chemistry Chemical Physics, 2013, 15, 18979.	1.3	150
8	Fe₂MnSi_xGe_{1â^'x}: influence thermoelectric properties of varying the germanium content. RSC Advances, 2014, 4, 39565-39571.	1.7	150
9	Thermoelectric properties for AA- and AB-stacking of a carbon nitride polymorph (C₃N₄). RSC Advances, 2014, 4, 63137-63142.	1.7	147
10	Ferroelectric polarization promoted bulk charge separation for highly efficient CO2 photoreduction of SrBi4Ti4O15. Nano Energy, 2019, 56, 840-850.	8.2	144
11	FP-APW+lo calculations of the elastic properties in zinc-blende III-P compounds under pressure effects. Computational Materials Science, 2009, 45, 474-479.	1.4	137
12	Spin-polarized Second Harmonic Generation from the Antiferromagnetic CaCoSO Single Crystal. Scientific Reports, 2017, 7, 46415.	1.6	128
13	Investigation of the Linear and Nonlinear Optical Susceptibilities of KTiOPO₄ Single Crystals: Theory and Experiment. Journal of Physical Chemistry B, 2010, 114, 16705-16712.	1.2	119
14	Thickness dependence of structural, electrical and optical behaviour of undoped ZnO thin films. Physica B: Condensed Matter, 2008, 403, 3326-3330.	1.3	116
15	Ab initio study of structural, electronic, elastic and high pressure properties of barium chalcogenides. Computational Materials Science, 2006, 38, 263-270.	1.4	106
16	Ab-initio calculations of Co-based diluted magnetic semiconductors Cd1â^'xCoxX (X=S, Se, Te). Journal of Magnetism and Magnetic Materials, 2010, 322, 3214-3222.	1.0	102
17	DFT calculation for elastic constants of orthorhombic structure within WIEN2K code: A new package (ortho-elastic). Journal of Alloys and Compounds, 2012, 543, 147-151.	2.8	100
18	Second order optical effects in Au nanoparticle-deposited ZnO nanocrystallite films. Nanotechnology, 2008, 19, 185709.	1.3	95

#	Article	IF	Citations
19	Theoretical study of mechanical, electronic, chemical bonding and optical properties of Ti2SnC, Zr2SnC, Hf2SnC and Nb2SnC. Computational Materials Science, 2009, 47, 491-500.	1.4	95
20	Band energy and thermoelectricity of filled skutterudites LaFe4Sb12 and CeFe4Sb12. Journal of Alloys and Compounds, 2007, 437, 39-46.	2.8	90
21	Ab-initio investigation of structural, electronic and optical properties for three phases of ZnO compound. Physica Status Solidi (B): Basic Research, 2007, 244, 3154-3167.	0.7	86
22	Variation of half metallicity and magnetism of Cd1â^'xCrxZ (Z=S, Se and Te) DMS compounds on reducing dilute limit. Journal of Magnetism and Magnetic Materials, 2013, 331, 1-6.	1.0	86
23	Electronic and optical properties of the1Tphases ofTiS2,TiSe2,andTiTe2. Physical Review B, 2003, 68, .	1.1	82
24	Calculated optical properties of2Hâ^'MoS2intercalated with lithium. Physical Review B, 2003, 68, .	1.1	80
25	Firstâ€principles calculations of structural, elastic and electronic properties of Ni₂MnZ (Z) Tj ETQq1 1 0.784314 rgBT /Ov	0.7	80
26	Exploration of the Electronic Structure of Monoclinic Î±-Eu₂(MoO₄)₃: DFT-Based Study and X-ray Photoelectron Spectroscopy. Journal of Physical Chemistry C, 2016, 120, 10559-10568.	1.5	80
27	Thermoelectric properties of a single graphene sheet and its derivatives. Journal of Materials Chemistry C, 2014, 2, 2346.	2.7	79
28	Structural, mechanical and electronic properties of sodium based fluoroperovskites NaXF3 (X=Mg,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50	1.9	79
29	Electronic structure, magnetism and robust half-metallicity of new quaternary Heusler alloy FeCrMnSb. Journal of Alloys and Compounds, 2013, 580, 201-204.	2.8	74
30	Coupling ferroelectric polarization and anisotropic charge migration for enhanced CO2 photoreduction. Applied Catalysis B: Environmental, 2021, 284, 119709.	10.8	74
31	Full-potential calculations of structural, elastic and electronic properties of MgAl2O4 and ZnAl2O4 compounds. Physics Letters, Section A: General, Atomic and Solid State Physics, 2005, 344, 271-279.	0.9	73
32	Structural and optical insights to enhance solar cell performance of CdS nanostructures. Energy Conversion and Management, 2014, 82, 238-243.	4.4	71
33	First-principles calculations of the elastic, electronic, and optical properties of the filled skutteruditesCeFe4P12andThFe4P12. Physical Review B, 2007, 75, .	1.1	66
34	First principles density functional calculations of half-metallic ferromagnetism in Zn1-xCrxS and Cd1-xCrxS. Current Opinion in Solid State and Materials Science, 2010, 14, 1-6.	5.6	65
35	Elastic, electronic and optical properties of cubic antiperovskites SbNCa3 and BiNCa3. Computational Materials Science, 2009, 46, 1051-1057.	1.4	64
36	Full-potential calculation of the structural, elastic, electronic and magnetic properties of XFeO3 (X=Sr and Ba) perovskite. Physica B: Condensed Matter, 2010, 405, 3515-3519.	1.3	64

#	Article	IF	Citations
37	Engineering oxygen vacancies towards self-activated BaLuAl_xZn_{4â^'x}O_{7â^'(1â^'x)/2}photoluminescent materials: an experimental and theoretical analysis. Physical Chemistry Chemical Physics, 2015, 17, 31188-31194.	1.3	64
38	An ab initio study of the electronic structure and optical properties of CdS1â^'Te alloys. Solar Energy, 2010, 84, 1979-1984.	2.9	63
39	Linear, nonlinear optical properties and birefringence of AgGaX2 (X=S, Se, Te) compounds. Physica B: Condensed Matter, 2005, 369, 243-253.	1.3	60
40	Visible-Light-Responsive SillÃ©n-Structured Mixed-Cationic CdBiO₂Br Nanosheets: Layer Structure Design Promoting Charge Separation and Oxygen Activation Reactions. Journal of Physical Chemistry C, 2018, 122, 2661-2672.	1.5	60
41	Theoretical investigation of the electronic properties, and first and second harmonic generation for cadmium chalcogenide. Journal of Chemical Physics, 2006, 124, 104707.	1.2	56
42	Role of titanium valence states in optical and electronic features of PbOâ€“Sb2O3â€“B2O3:TiO2 glass alloys. Journal of Alloys and Compounds, 2009, 482, 283-297.	2.8	56
43	Elastic properties and bonding of the AgGaSe2 chalcopyrite. Physica B: Condensed Matter, 2010, 405, 3658-3664.	1.3	56
44	Emergence of half metallicity in Cr-doped GaP dilute magnetic semiconductor compound within solubility limit. Journal of Alloys and Compounds, 2012, 536, 214-218.	2.8	56
45	Effect of U on the Electronic Properties of Neodymium Gallate (NdGaO₃): Theoretical and Experimental Studies. Journal of Physical Chemistry B, 2009, 113, 15237-15242.	1.2	53
46	The under-pressure behaviour of mechanical, electronic and optical properties of calcium titanate and its ground state thermoelectric response. Philosophical Magazine, 2017, 97, 1884-1901.	0.7	53
47	Theoretical investigation of the electronic and optical properties of ZrX2 (X=S, Se and Te). Physica B: Condensed Matter, 2004, 353, 230-237.	1.3	52
48	First-Principles Calculations of Structural, Elastic, Electronic, and Optical Properties of Perovskite-type KMgH₃ Crystals: Novel Hydrogen Storage Material. Journal of Physical Chemistry B, 2011, 115, 2836-2841.	1.2	52
49	Specific features in the band structure and linear and nonlinear optical susceptibilities ofLa2CaB10O19crystals. Physical Review B, 2007, 75, .	1.1	51
50	FP-APW+lo study of the elastic, electronic and optical properties of the filled skutterudites CeFe4As12 and CeFe4Sb12. Current Opinion in Solid State and Materials Science, 2009, 13, 105-111.	5.6	51
51	First-principle calculations of the linear and nonlinear optical response for GaX (X = As, Sb, P). European Physical Journal B, 2005, 47, 503-508.	0.6	50
52	First-principles study of spin-polarized electronic band structures in ferromagnetic Zn1â^'xTMxS (TM=Fe, Co and Ni). Journal of Alloys and Compounds, 2010, 508, 245-250.	2.8	50
53	Ab initio method of optical investigations of CdS1â^'Te alloys under quantum dots diameter effect. Solar Energy, 2015, 115, 33-39.	2.9	50
54	Two symmetric n-type interfaces SrTiO3/LaAlO3 in perovskite: Electronic properties from density functional theory. Journal of Applied Physics, 2016, 119, .	1.1	50

#	Article	IF	Citations
55	Mechanical and thermodynamical properties of hexagonal compounds at optimized lattice parameters from two-dimensional search of the equation of state. RSC Advances, 2014, 4, 57903-57915.	1.7	49
56	Insight into the physical properties of the inter-metallic titanium-based binary compounds. European Physical Journal Plus, 2021, 136, 1.	1.2	49
57	Linear and nonlinear optical susceptibilities for a novel borate oxide BaBiBO4: Theory and experiment. Journal of Solid State Chemistry, 2008, 181, 789-795.	1.4	48
58	Structural, chemical bonding, electronic and magnetic properties of KMF3 (M = Mn, Fe, Co, Ni) compounds. Computational Materials Science, 2014, 85, 402-408.	1.4	48
59	Pressureâ€dependent <scp>elastoâ€mechanical</scp> stability and thermoelectric properties of <scp> MYbF ₃ </scp> (M = Rb, Cs) materials for renewable energy. International Journal of Energy Research, 2021, 45, 8711-8723.	2.2	48
60	Electronic, linear, and nonlinear optical properties of III-V indium compound semiconductors. Journal of Chemical Physics, 2006, 125, 034710.	1.2	47
61	Effect of increasing tellurium content on the electronic and optical properties of cadmium selenide telluride alloys CdSe1â^'xTex: An ab initio study. Journal of Alloys and Compounds, 2011, 509, 6737-6750.	2.8	47
62	Electronic spectral parameters and IR nonlinear optical features of novel Ag0.5Pb1.75GeS4 crystal. Journal of Crystal Growth, 2012, 354, 142-146.	0.7	47
63	Genesis of magnetism in graphene/MoS2 van der Waals heterostructures via interface engineering using Cr-adsorption. Journal of Alloys and Compounds, 2021, 859, 157776.	2.8	47
64	Electronic Structure of Quaternary Chalcogenide Ag₂In₂Ge(Si)S₆ Single Crystals and the Influence of Replacing Ge by Si: Experimental X-Ray Photoelectron Spectroscopy and X-Ray Diffraction Studies and Theoretical Calculations. Science of Advanced Materials, 2013, 5, 316-327.	0.1	46
65	Thermoelectric properties of Nowotnyâ€"Juza NaZnX (X = P, As and Sb) compounds. Computational Materials Science, 2015, 96, 90-95.	1.4	46
66	Co2YZ (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
67	Band structure and optical response of2Hâ^'MoX2compounds (X=S, Se, and Te). Physical Review B, 2005, 71, .	1.1	45
68	Ab initio calculations of the electronic, linear and nonlinear optical properties of zinc chalcogenides. Physica B: Condensed Matter, 2007, 388, 34-42.	1.3	45
69	Spin-Polarized Structural, Electronic, and Magnetic Properties of Diluted Magnetic Semiconductors Cd_{1â^'x}Mn_xS and Cd_{1â^'x}Mn_xSe in Zinc Blende Phase. Journal of Physical Chemistry A, 2009, 113, 6022-6027.	1.1	45
70	Dispersion of linear and non-linear optical susceptibilities for amino acid 2-aminopropanoic CH3CH(NH2)COOH single crystals: experimental and theoretical investigations. Journal of Materials Chemistry, 2011, 21, 17219.	6.7	45
71	Density functional study of optical properties of beryllium chalcogenides compounds in nickel arsenide B8 structure. Physica B: Condensed Matter, 2012, 407, 286-296.	1.3	45
72	Theoretical investigations of NiTiSn and CoVSn compounds. Journal of Physics and Chemistry of Solids, 2012, 73, 975-981.	1.9	44

#	Article	IF	Citations
73	Accounting oxygen vacancy for half-metallicity and magnetism in Fe-doped CeO2 dilute magnetic oxide. Computational Materials Science, 2013, 74, 114-118.	1.4	44
74	First and second harmonic generation of the optical susceptibilities for the non-centro-symmetric orthorhombic AgCd₂GaS₄. Journal of Physics Condensed Matter, 2008, 20, 325234.	0.7	43
75	Acentric Nonlinear Optical 2,4-Dihydroxyl Hydrazone Isomorphic Crystals with Large Linear, Nonlinear Optical Susceptibilities and Hyperpolarizability. Journal of Physical Chemistry B, 2012, 116, 4677-4683.	1.2	43
76	Specific features of electronic structures and optical susceptibilities of molybdenum oxide. RSC Advances, 2015, 5, 22044-22052.	1.7	43
77	Active photocatalytic water splitting solar-to-hydrogen energy conversion: Chalcogenide photocatalyst Ba2ZnSe3 under visible irradiation. Applied Catalysis B: Environmental, 2018, 221, 17-26.	10.8	42
78	Electro-structural correlations, elastic and optical properties among the nanolaminated ternary carbides Zr2AC. Solid State Sciences, 2010, 12, 887-898.	1.5	41
79	GGA+U studies of the cubic perovskites BaMO3 (M=Pr, Th and U). Physica B: Condensed Matter, 2013, 410, 217-221.	1.3	41
80	Several features of nonlinear optical susceptibilities of LiGaX2 (X=S, Se) ternary compounds. Journal of Alloys and Compounds, 2009, 473, 20-24.	2.8	40
81	Linear and Nonlinear Optical Susceptibilities of 3-Phenylamino-4-phenyl-1,2,4-triazole-5-thione. Journal of Physical Chemistry B, 2010, 114, 1815-1821.	1.2	40
82	Quantum dots in photocatalytic applications: efficiently enhancing visible light photocatalytic activity by integrating CdO quantum dots as sensitizers. Physical Chemistry Chemical Physics, 2017, 19, 24915-24927.	1.3	40
83	Ab-initio study of the structural, linear and nonlinear optical properties of CdAl2Se4 defect-chalcopyrite. Journal of Solid State Chemistry, 2010, 183, 46-51.	1.4	39
84	Linear and Nonlinear Optical Susceptibilities and the Hyperpolarizability of Borate LiBaB₉O₁₅ Single-Crystal: Theory and Experiment. Journal of Physical Chemistry B, 2013, 117, 14141-14150.	1.2	39
85	Strain effect on the electronic and optical properties of 2D Tetrahexcarbon: a DFT-based study. Indian Journal of Physics, 2021, 95, 2365-2373.	0.9	39
86	Structural, electronic, elastic, and magnetic properties of <scp> NaQF ₃ </scp> (QÂ=Âag, Pb,) Tj ETQq0 0 0 rgBT /Overlock 2022, 46, 2446-2453.	2.2	39
87	Influence of Replacing Si by Ge in the Chalcogenide Quaternary Sulfides Ag2In2Si(Ge)S6 on the Chemical Bonding, Linear and Nonlinear Optical Susceptibilities, and Hyperpolarizability. Journal of Physical Chemistry B, 2013, 117, 2545-2553.	1.2	38
88	Theoretical investigation of the structural, electronic, magnetic and elastic properties of binary cubic C15-Laves phases TbX2 (XÂ=ÂCo and Fe). Journal of Alloys and Compounds, 2016, 689, 885-893.	2.8	38
89	Electronic structure and optical properties of 1T-TiS2 and lithium intercalated 1T-TiS2 for lithium batteries. Journal of Chemical Physics, 2008, 129, 074706.	1.2	37
90	Calculation of the lattice constant of hexagonal compounds with two dimensional search of equation of state and with semilocal functionals a new package (2D-optimize). Journal of Alloys and Compounds, 2013, 555, 362-366.	2.8	37

#	Article	IF	Citations
91	Structural, elastic, electronic, magnetic, optical, and thermoelectric properties of the diamond-like quaternary semiconductor CuMn2InSe4. Journal of Superconductivity and Novel Magnetism, 2020, 33, 1091-1102.	0.8	37
92	Ab-initio calculation of structural, electronic, and optical characterizations of the intermetallic trialuminides ScAl3 compound. Journal of Solid State Chemistry, 2010, 183, 1290-1296.	1.4	36
93	Optical Spectra and Band Structure of Ag_xGa_xGe_{1â€“x}Se₂ (x = 0.333,) Tj ETQq1 1 0.784314 15220-15231.	1.2	36
94	Adsorbing H2S onto a single graphene sheet: A possible gas sensor. Journal of Applied Physics, 2014, 116, .	1.1	36
95	Photoinduced effects in TiO2 nanocrystalline films with different morphology. Journal of Alloys and Compounds, 2010, 508, 599-605.	2.8	35
96	Evidence of Coulomb correction and spinâ€“orbit coupling in rare-earth dioxides CeO2, PrO2 and TbO2: An ab initio study. Journal of Magnetism and Magnetic Materials, 2012, 324, 1397-1405.	1.0	35
97	Comparative study of Fe doped ZnO based diluted and condensed magnetic semiconductors in wurtzite and zinc-blende structures by first-principles calculations. Materials Science in Semiconductor Processing, 2016, 43, 123-128.	1.9	35
98	Novel borate CsZn2B3O7 single crystal with large efficient second harmonic generation in deep-ultraviolet spectral range. Journal of Alloys and Compounds, 2017, 722, 438-444.	2.8	35
99	Electronic, optical and bonding properties of MgYZ2 (Y=Si, Ge; Z=N, P) chalcopyrites from first principles. Materials Science in Semiconductor Processing, 2014, 26, 79-86.	1.9	34
100	Comparative first-principles calculations of the electronic, optical, elastic and thermodynamic properties of XCaF3 (XÂ=ÂK, Rb, Cs) cubic perovskites. Materials Chemistry and Physics, 2017, 188, 39-48.	2.0	34
101	First-Principles Study on the Structural, Electronic, Magnetic and Thermodynamic Properties of Full Heusler Alloys Co2VZ (ZÂ=ÂAl, Ga). Journal of Electronic Materials, 2017, 46, 130-142.	1.0	34
102	Full-potential calculations of the electronic and optical properties for 1T and 2H phases of TaS2 and TaSe2. Physica B: Condensed Matter, 2005, 358, 158-165.	1.3	33
103	Photoinduced effects in l-alanine crystals. Materials Letters, 2010, 64, 1957-1959.	1.3	33
104	Bismuth-containing semiconductors: Linear and nonlinear optical susceptibilities of GaAs1â^'xBix alloys. Journal of Alloys and Compounds, 2011, 509, 9685-9691.	2.8	33
105	First-principles study of structural stabilities, elastic and electronic properties of transition metal monocarbides (TMCs) and mononitrides (TMNs). Materials Chemistry and Physics, 2013, 143, 93-108.	2.0	33
106	External temperature and pressure effects on thermodynamic properties and mechanical stability of yttrium chalcogenides YX (X=S, Se and Te). Physica B: Condensed Matter, 2013, 428, 78-88.	1.3	33
107	Third harmonic generation process in Al doped ZnO thin films. Journal of Alloys and Compounds, 2014, 584, 7-12.	2.8	33
108	Synthesis, Structural, Thermal, and Electronic Properties of Palmierite-Related Double Molybdate Î±-Cs₂Pb(MoO₄)₂. Inorganic Chemistry, 2017, 56, 3276-3286.	1.9	33

#	Article	IF	Citations
109	Insight into crystal-structure dependent charge separation and photo-redox catalysis: A combined experimental and theoretical study on Bi(IO3)3 and BiOIO3. Applied Surface Science, 2018, 458, 129-138.	3.1	33
110	Investigation of the electronic properties, first and second harmonic generation for AXIIIBXV zinc-blende semiconductors. Physica B: Condensed Matter, 2007, 395, 143-150.	1.3	32
111	Electronic properties of chalcopyrite CuAlX2(X=S,Se,Te) compounds. Solid State Communications, 2008, 145, 571-576.	0.9	32
112	FP-APW+lo calculations of the electronic and optical properties of alkali metal sulfides under pressure. Journal of Physics Condensed Matter, 2009, 21, 095404.	0.7	32
113	Calculated optical properties of GaX (X=P, As, Sb) under hydrostatic pressure. Applied Physics A: Materials Science and Processing, 2011, 104, 1159-1167.	1.1	32
114	Electronic band structure and specific features of AA- and AB-stacking of carbon nitride (C3N4): DFT calculation. RSC Advances, 2014, 4, 6957.	1.7	32
115	Alkali-metal/alkaline-earth-metal fluorine beryllium borate NaSr3Be3B3O9F4with large nonlinear optical properties in the deep-ultraviolet region. Journal of Applied Physics, 2015, 117, 085703.	1.1	32
116	Electronic and optical properties of pentagonal-B₂C monolayer: A first-principles calculation. International Journal of Modern Physics B, 2017, 31, 1750044.	1.0	32
117	Ab initio calculations of the electronic and optical properties of 1T-HfX2 compounds. Physica B: Condensed Matter, 2005, 363, 25-31.	1.3	31
118	Structural, electronic and optical properties of fluorite-type compounds. European Physical Journal B, 2005, 47, 63-70.	0.6	31
119	First-principles study of the optical properties of PbFX (X = Cl, Br, I) compounds in its matlockite-type structure. European Physical Journal B, 2007, 60, 463-468.	0.6	31
120	Experimental and theoretical investigations of the first and second order optical susceptibilities of BiB3O6 single crystal. Applied Physics A: Materials Science and Processing, 2008, 91, 451-457.	1.1	31
121	X-ray diffraction and optical properties of a noncentrosymmetric borate CaBiGaB2O7. Journal of Chemical Physics, 2008, 129, 204111.	1.2	31
122	Full potential study of the elastic, electronic, and optical properties of spinels MgIn2S4 and CdIn2S4 under pressure effect. Journal of Solid State Chemistry, 2010, 183, 2818-2825.	1.4	31
123	Dispersion of Linear, Nonlinear Optical Susceptibilities and Hyperpolarizability of C₁₁H₈N₂O (o-Methoxydicyanovinylbenzene) Crystals. Journal of Physical Chemistry B, 2012, 116, 13338-13343.	1.2	31
124	Structural and electronic properties of GaN x As1â^'x alloys. Applied Physics A: Materials Science and Processing, 2012, 106, 687-696.	1.1	31
125	Analytical investigations of CdS nanostructures for optoelectronic applications. Optik, 2015, 126, 5109-5114.	1.4	31
126	The influence of oxygen vacancies on the linear and nonlinear optical properties of Pb₇O(OH)₃(CO₃)₃(BO₃). RSC Advances, 2017, 7, 14752-14760.	1.7	31

#	Article	IF	Citations
127	Noncentrosymmetric Sulfide Oxide MZnSO (M = Ca or Sr) with Strongly Polar Structure as Novel Nonlinear Crystals. Journal of Physical Chemistry C, 2019, 123, 27172-27180.	1.5	31
128	Dielectric absorption correlated to ferromagnetic behavior in (Cr, Ni)-codoped 4Hâ€“SiC for microwave applications. Journal of Molecular Structure, 2022, 1248, 131462.	1.8	31
129	Effect of cation substitution on electronic band structure of ZnGeAs2 pnictides: A mBJLDA approach. Journal of Alloys and Compounds, 2012, 518, 74-79.	2.8	30
130	Electronic structure and optical properties of In2X2O7 (X=Si, Ge, Sn) from direct to indirect gap: An ab initio study. Computational Materials Science, 2013, 78, 91-97.	1.4	30
131	The density functional study of electronic structure, electronic charge density, linear and nonlinear optical properties of single crystal alpha-LiAlTe2. Journal of Alloys and Compounds, 2014, 592, 92-99.	2.8	30
132	Linear and nonlinear optical properties for AA and AB stacking of carbon nitride polymorph (C₃N₄). RSC Advances, 2014, 4, 11967-11974.	1.7	30
133	Quest for magnetism in graphene via Cr- and Mo-doping: A DFT approach. Physica E: Low-Dimensional Systems and Nanostructures, 2016, 78, 35-40.	1.3	30
134	Sulfide oxide XZnSO (X = Ca or Sr) as novel active photocatalytic water splitting solar-to-hydrogen energy conversion. Applied Catalysis B: Environmental, 2018, 225, 273-283.	10.8	30
135	Prediction study of the structural and elastic properties for the cubic skutterudites LaFe4A12 (AÂ= ÂP,) Tj ETQq1 1 0.784314 rgBT /Ov	0.9	29
136	Prediction study of the structural, elastic and high pressure properties of Yttrium chalcogenide. Computational Materials Science, 2010, 49, 372-377.	1.4	29
137	FP-LAPW investigation of structural, electronic, linear and nonlinear optical properties of ZnIn2Te4 defect-chalcopyrite. Computational Materials Science, 2010, 50, 651-655.	1.4	29
138	Structural, Elastic, Electronic and Optical Properties of Cu₃TMSe₄ (TM = V,) Tj ETQq0 0 0 rgBT /Overlock 10 T 5, 97-106.	0.1	29
139	Investigation of electronic structure and optical properties of MgAl2O4: DFT approach. Optical Materials, 2014, 37, 322-326.	1.7	29
140	Electronic, optical, and thermoelectric properties of Fe2+xV1â^'xAl. AIP Advances, 2017, 7, .	0.6	29
141	MgH2 and LiH metal hydrides crystals as novel hydrogen storage material: Electronic structure and optical properties. International Journal of Hydrogen Energy, 2013, 38, 11946-11954.	3.8	28
142	Transport properties of mixed CuAl(S1â^'xSex)2 as promising thermoelectric crystalline materials. Journal of Physics and Chemistry of Solids, 2015, 78, 46-52.	1.9	28
143	First-principles investigation of the optical properties for rocksalt mixed metal oxide Mg Zn1â^'O. Materials Chemistry and Physics, 2016, 182, 182-189.	2.0	28
144	Phase transition of LaX (XÂ= ÂP, As, Sb and Bi) at high pressure: Theoretical investigation of the structural and electronic properties. Solid State Communications, 2008, 148, 139-144.	0.9	27

#	Article	IF	Citations
145	Electronic properties of orthorhombic LiGaS2 and LiGaSe2. Applied Physics A: Materials Science and Processing, 2009, 94, 315-320.	1.1	27
146	First principles calculations of electronic structure and magnetic properties of Cr-based magnetic semiconductors Al1â^'xCrxX (X=N, P, As, Sb). Journal of Solid State Chemistry, 2010, 183, 242-249.	1.4	27
147	Bismuth in gallium arsenide: Structural and electronic properties of GaAs1â^'xBix alloys. Journal of Solid State Chemistry, 2012, 186, 47-53.	1.4	27
148	Thermoelectric properties of highly-mismatched alloys of GaN_xAs_{1â^'x}from first- to second-principles methods: energy conversion. RSC Advances, 2016, 6, 72286-72294.	1.7	27
149	Synthesis and Characterization of Cu2CdSnS4 Quaternary Alloy Nanostructures. International Journal of Electrochemical Science, 2018, 13, 6693-6707.	0.5	27
150	First principles study of the elastic properties in X2S (X=Li, Na, K and Rb) compounds under pressure effect. Solid State Communications, 2008, 147, 178-182.	0.9	26
151	X-ray photoelectron spectra and the electronic band structure for non-centrosymmetric Bi2ZnB2O7 nonlinear single crystal. Current Opinion in Solid State and Materials Science, 2008, 12, 26-31.	5.6	26
152	NaMgH3 a perovskite-type hydride as advanced hydrogen storage systems: Electronic structure features. International Journal of Hydrogen Energy, 2015, 40, 16383-16390.	3.8	26
153	Transport properties of g-BC₃and t-BC₃phases. RSC Advances, 2015, 5, 33632-33638.	1.7	26
154	Structural, electronic and magnetic properties of new full Heusler alloys Rh2CrZ (Zâ€¯=â€¯Al, Ga, In): First-principles calculations. Chinese Journal of Physics, 2019, 59, 281-290.	2.0	26
155	Electronic band structure of AgCd2GaS4: theory and experiment. Journal of Physics Condensed Matter, 2008, 20, 325213.	0.7	25
156	Electronic Band Structure and Optical Properties of Sr_{n+1}Ti_nO_{3n+1} Ruddlesdenâ€“Popper Homologous Series. Japanese Journal of Applied Physics, 2008, 47, 5516.	0.8	25
157	Absorption and photoconductivity spectra of Ag2GeS3 crystal: Experiment and theory. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2012, 93, 274-279.	2.0	25
158	Theoretical investigation of band gap and optical properties of ZnO 1â^' x Te x alloys (x = 0, 0.25, 0.5, 0.75) Tj ETQq0 0 0 rgBT /Overlock	1.4	25
159	Electronic and optical properties of chair-like and boat-like graphane. RSC Advances, 2014, 4, 37411-37418.	1.7	25
160	Spectral emission properties of 4-aryloxy-3-methyl-1-phenyl-1H-pyrazolo[3,4-b]quinolines. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2009, 73, 281-285.	2.0	24
161	Density functional calculations of the electronic structure of 3-phenylamino-4-phenyl-1,2,4-triazole-5-thione. Physical Chemistry Chemical Physics, 2010, 12, 2975.	1.3	24
162	Optical and photoconductivity spectra of novel Ag2In2SiS6 and Ag2In2GeS6 chalcogenide crystals. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2012, 91, 48-50.	2.0	24

#	Article	IF	Citations
163	Structural investigations through cobalt effect on ZnO nanostructures. Optik, 2016, 127, 10102-10107.	1.4	24
164	Electronic and optical properties of paratellurite TeO2 under pressure: A first-principles calculation. Optik, 2017, 139, 9-15.	1.4	24
165	Piezooptical effects in the tellurite glasses doped by europium and gold. Optics Communications, 2008, 281, 3721-3725.	1.0	23
166	X-ray Photoelectron Spectrum and Electronic Properties of a Noncentrosymmetric Chalcopyrite Compound HgGa2S4: LDA, GGA, and EV-GGA. Journal of Physical Chemistry B, 2009, 113, 5803-5808.	1.2	23
167	Photoinduced nonlinear optical effects in the Pr doped BiB3O6 glass nanoparticles incorporated into the polymer matrices. Journal of Alloys and Compounds, 2009, 485, 29-32.	2.8	23
168	Electronic band structure and specific features of Sm2NiMnO6 compound: DFT calculation. Journal of Magnetism and Magnetic Materials, 2013, 342, 80-86.	1.0	23
169	Two haloid borate crystals with large nonlinear optical response. Physical Chemistry Chemical Physics, 2017, 19, 18416-18425.	1.3	23
170	Electronic and optical properties of2Hâˆ’WSe2intercalated with copper. Physical Review B, 2003, 68, .	1.1	22
171	UV-excited piezo-optical effects in oxide nanocrystals incorporated into PMMA matrices. Acta Materialia, 2008, 56, 5677-5684.	3.8	22
172	First principles study of structural, electronic and magnetic properties of Mg1âˆ’xMnxTe alloys. Journal of Alloys and Compounds, 2011, 509, 8137-8143.	2.8	22
173	Fluorescent and nonlinear optical features of CdTe quantum dots. Journal of Materials Science: Materials in Electronics, 2012, 23, 546-550.	1.1	22
174	Density of electronic states and dispersion of optical functions of defect chalcopyrite CdGa2X4 (X=S,) Tj ETQq0 0 0 rgBT /Overlock 10 T	2.7	22
175	Thermoelectric properties of fully hydrogenated graphene: Semi-classical Boltzmann theory. Journal of Applied Physics, 2015, 117, .	1.1	22
176	Transport properties of Co-based Heusler compounds Co2VAl and Co2VGa: spin-polarized DFT+U. RSC Advances, 2016, 6, 54001-54012.	1.7	22
177	Strong second harmonic generation in LiInX2 (X=Se, Te) chalcopyrite crystals as explored by first-principles methods. Journal of Alloys and Compounds, 2016, 675, 355-363.	2.8	22
178	Role of spinâ€“orbit interaction on the nonlinear optical response of CsPbCO₃F using DFT. Physical Chemistry Chemical Physics, 2017, 19, 31255-31266.	1.3	22
179	Specific features of 3, 6-bis (4-hydroxy phenyl)-piperazine-2, 5-dione (BHPPD) diphenolic monomer and compered with toxic industrial bisphenol-A (BPA): DFT calculation. Materials Chemistry and Physics, 2019, 236, 121780.	2.0	22
180	Photoinduced non-linear optical effects in lanthanum calcium borate single crystals. Journal of Materials Science, 2006, 41, 1927-1932.	1.7	21

#	Article	IF	Citations
181	Energy band structure and density of states for BaBiBO4 nonlinear optical crystal. Journal of Alloys and Compounds, 2008, 460, 99-102.	2.8	21
182	First-principles study of structural, electronic, linear and nonlinear optical properties of Ga2PSb ternary chalcopyrite. European Physical Journal B, 2009, 72, 361-366.	0.6	21
183	FP-APW+lo study of the elastic, electronic and optical properties for the cubic antiperovskite ANSr3 (A=As, Sb and Bi) under pressure effect. Physica B: Condensed Matter, 2010, 405, 1894-1900.	1.3	21
184	Investigated optical studies of Si quantum dot. Solar Energy, 2011, 85, 2283-2287.	2.9	21
185	Dispersion of the linear and nonlinear optical susceptibilities of disilver germanium sulfide from DFT calculations. Journal of Materials Science, 2013, 48, 1955-1965.	1.7	21
186	Synthesis, Crystal Structure, and Optical Gap of Two-Dimensional Halide Solid Solutions CsPb₂(Cl_{1â€“x}Br_x)₅. Inorganic Chemistry, 2018, 57, 9531-9537.	1.9	21
187	Electronic structure, linear, nonlinear optical susceptibilities and birefringence of CuInX2(X = S, Se,) Tj ETQq1 1 0.784314 rgBT /Overlock	0.9	20
188	Band structure features of nonlinear optical yttrium aluminium borate crystal. Solid State Sciences, 2008, 10, 1445-1448.	1.5	20
189	Birefringence, linear and nonlinear second-order optical susceptibilities of a noncentrosymmetric chalcopyrite compound HgGa2S4. Current Opinion in Solid State and Materials Science, 2008, 12, 14-18.	5.6	20
190	Linear and nonlinear optical susceptibilities and hyperpolarizability of borate LiNaB4O7 single crystals: Theory and experiment. Journal of Applied Physics, 2012, 112, .	1.1	20
191	First and second harmonic generation of the XAl2Se4 (X=Zn,Cd,Hg) defect chalcopyrite compounds. Physica B: Condensed Matter, 2012, 407, 3760-3766.	1.3	20
192	X-ray photoelectron spectrum, X-ray diffraction data, and electronic structure of chalcogenide quaternary sulfide Ag2In2GeS6: experiment and theory. Journal of Materials Science, 2013, 48, 1342-1350.	1.7	20
193	Electronic structure, charge density, and chemical bonding properties of C11H8N2O o-methoxydicyanovinylbenzene (DIVA) single crystal. Journal of Materials Science, 2013, 48, 5157-5162.	1.7	20
194	Tuning Fermi level of Cr2CoZ (Z=Al and Si) inverse Heusler alloys via Fe-doping for maximum spin polarization. Journal of Magnetism and Magnetic Materials, 2014, 370, 81-86.	1.0	20
195	Half-metallic ferromagnetism in Al1â^'xCrxP and superlattices (AlP)n/(CrP)m by density functional calculations. Superlattices and Microstructures, 2014, 65, 195-205.	1.4	20
196	Thermoelectric properties of Sr+1Ti O3+1 (n=1, 2, 3, â^ž) Ruddlesdenâ€“Popper Homologous Series. Renewable Energy, 2015, 76, 36-44.	4.3	20
197	Structural, optical and electrical properties of Cu2Zn1â^'xCdxSnS4 quinternary alloys nanostructures deposited on porous silicon. Microsystem Technologies, 2016, 22, 2893-2900.	1.2	20
198	Magnetism and magnetocrystalline anisotropy of tetragonally distorted L10-FeNi: N alloy. Journal of Alloys and Compounds, 2020, 835, 155325.	2.8	20

#	Article	IF	Citations
199	Specific features of second order optical susceptibilities for a complex borate crystal Bi2ZnB2O7: Experiment and theory. Current Opinion in Solid State and Materials Science, 2007, 11, 33-39.	5.6	19
200	The linear and nonlinear optical properties of WSxSe2â^'x (x=0.5, 1.5, and 2.0). Physica B: Condensed Matter, 2007, 393, 88-93.	1.3	19
201	Structural, electronic and optical properties of AgI under pressure. Physics Letters, Section A: General, Atomic and Solid State Physics, 2008, 372, 2502-2508.	0.9	19
202	Optical susceptibilities of Na3La9O3(BO3)8, ternary oxyborate nonlinear single crystal: theory and experiment. Journal of Physics Condensed Matter, 2008, 20, 145209.	0.7	19
203	Copper-Intercalated TiS₂: Electrode Materials for Rechargeable Batteries as Future Power Resources. Journal of Physical Chemistry A, 2009, 113, 1635-1645.	1.1	19
204	The effect of chalcogen atom on the structural, elastic, and highâ€pressure properties of XY compounds (Xâ€‰=â€‰La, Ce, Eu, and Yâ€‰=â€‰S, Se, and Te): An ab initio study. Physica Status Solidi (B): Basic Research, 2012, 249, 18-28.	1.5	19
205	Disorder dependent half-metallicity in Mn2CoSi inverse Heusler alloy. Journal of Solid State Chemistry, 2013, 208, 71-77.	1.4	19
206	Generating magnetic response and half-metallicity in GaP via dilute Ti-doping for spintronic applications. Journal of Alloys and Compounds, 2015, 649, 184-189.	2.8	19
207	Mechanical stability and optoelectronic behavior of BeXP2 (X=Si and Ge) chalcopyrite. Chinese Journal of Physics, 2020, 64, 174-182.	2.0	19
208	Structural and electronic properties of bulk GaP and AlP and their superlattices. Superlattices and Microstructures, 2011, 49, 132-143.	1.4	18
209	Simulation of Brillouin and Rayleigh scattering in distributed fibre optic for temperature and strain sensing application. Sensors and Actuators A: Physical, 2013, 190, 191-196.	2.0	18
210	Electrical behaviour of MEH-PPV based diode and transistor. Progress in Biophysics and Molecular Biology, 2013, 113, 289-294.	1.4	18
211	Highly desirable semiconducting materials for mid-IR optoelectronics: Dilute bismide InAs1â^'Bi alloys. Materials Research Bulletin, 2017, 95, 588-596.	2.7	18
212	Preparation, structure and photoluminescence properties of SiO2/ZnO nanocables via electrospinning and vapor transport deposition. Materials Letters, 2008, 62, 2088-2091.	1.3	17
213	Optically stimulated non-linear optics effects in semiconducting nano-crystallites. Physica E: Low-Dimensional Systems and Nanostructures, 2010, 42, 1769-1771.	1.3	17
214	Surface modification via wet chemical etching of single-crystalline silicon for photovoltaic application. Progress in Biophysics and Molecular Biology, 2013, 113, 327-332.	1.4	17
215	Electronic and optical properties of the SiB2O4 (B=Mg, Zn, and Cd) spinel oxides: An ab initio study with the Tranâ€“Blaha-modified Beckeâ€“Johnson density functional. Physica B: Condensed Matter, 2014, 443, 24-34.	1.3	17
216	Dispersion of the second harmonic generation from CdGa2X4 (X=S, Se) defect chalcopyrite: DFT calculations. Journal of Alloys and Compounds, 2014, 595, 125-130.	2.8	17

#	Article	IF	Citations
217	Novel photocatalytic water splitting solar-to-hydrogen energy conversion: CdLa₂S₄and CdLa₂Se₄ternary semiconductor compounds. Physical Chemistry Chemical Physics, 2018, 20, 8848-8858.	1.3	17
218	1,4-dialkoxy-2,5-bis[2-(thien-2-yl)ethenyl]benzenes as promising materials for laser optical limiters. Laser Physics, 2008, 18, 1056-1069.	0.6	16
219	Second harmonic generation from thick leaves using the two-photon laser scanning microscope. Micron, 2009, 40, 455-462.	1.1	16
220	Second harmonic imaging of chloroplasts using the two-photon laser scanning microscope. Micron, 2009, 40, 378-385.	1.1	16
221	Dispersion of Linear and Nonlinear Optical Susceptibilities in Calcium Neodymium Oxyborate Ca₄NdO(BO₃)₃â”LDA versus GGA. Journal of Physical Chemistry A, 2009, 113, 1614-1622.	1.1	16
222	FIRST PRINCIPLES STUDY OF THE STRUCTURAL, ELASTIC AND ELECTRONIC PROPERTIES OF Ti₂InC and Ti₂InN. Modern Physics Letters B, 2011, 25, 747-761.	1.0	16
223	Structural properties and bonding nature of 3-methyl-4-phenyl-5-(2-pyridyl)-1,2,4-triazole single crystal. Materials Chemistry and Physics, 2011, 130, 458-465.	2.0	16
224	Structural, electronic properties and charge density distribution of the LiNaB4O7: Theory and experiment. Materials Chemistry and Physics, 2012, 137, 346-352.	2.0	16
225	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
226	A novel photocatalytic water splitting solar-to-hydrogen energy conversion: Non-centro-symmetric borate CsZn2B3O7 photocatalyst. Journal of Alloys and Compounds, 2018, 741, 1258-1268.	2.8	16
227	Optoelectronic and transport properties of Rb/ <scp> Cs ₂ TeI ₆ </scp> defective perovskites for green energy applications. International Journal of Energy Research, 2021, 45, 8448-8455.	2.2	16
228	Influence of Tm⁺³concentration on the non-linear optical effects of the BiB₃O₆â€‰:â€‰Tm³⁺glass nanoparticle-doped polymer. Journal Physics D: Applied Physics, 2010, 43, 015103.	2.3	15
229	Electronic structure, chemical bonding features, and electron charge density of the double-cubane single crystal [Sb7S8Br2](AlCl4)3. Applied Physics Letters, 2011, 98, 201903.	1.5	15
230	Density functional theory calculation of the optical properties and topological analysis of the electron density of MBi2B2O7 (Mâ€‰=â€‰Ca,Zn) compounds. Journal of Applied Physics, 2013, 113, .	1.1	15
231	Enhanced magnetic response and metallicity in AB stacked bilayer graphene via Cr-doping. Journal of Alloys and Compounds, 2015, 649, 1300-1305.	2.8	15
232	Photocatalytic water splitting solar-to-hydrogen energy conversion: Perovskite-type hydride XBeH3 (X) Tj ETQq0 0 0 rgBT /Overlock 10 T	3.1	15
233	Fabrication and Characterization of a p-AgO/PSi/n-Si Heterojunction for Solar Cell Applications. Silicon, 2018, 10, 371-376.	1.8	15
234	Pressure induced physical variations in the lead free fluoropervoskites XYF3 (X=K, Rb, Ag; Y=Zn, Sr,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 5	1.7	15

#	Article	IF	Citations
235	Density functional theory based study of the physical properties of cesium based cubic halide perovskites <scp> CsHgX ₃ </scp> (Xâ•F and Cl). International Journal of Energy Research, 2022, 46, 2467-2476.	2.2	15
236	Optical second harmonic generation in Yttrium Aluminum Borate single crystals (theoretical) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 702 T	0.9	14
237	Optical properties of the alkaline-earth fluorohalides matlockite-type structure SrFX (X=Cl, Br, I) compounds. Physica B: Condensed Matter, 2008, 403, 711-716.	1.3	14
238	Novel nonlinear optical materials based on dihydropyridine organic chromophore deposited on mica substrate. Journal of Materials Science: Materials in Electronics, 2009, 20, 1073-1077.	1.1	14
239	Optical features of calcium neodymium oxyborate Ca4NdO(BO3)3 doped by Yb3+. Journal of Alloys and Compounds, 2009, 481, 14-16.	2.8	14
240	Ab Initio Calculation of the Electronic Band Structure, Density of States and Optical Properties of Î±-2-Methyl-1-nitroisothiourea. Journal of Physical Chemistry B, 2009, 113, 12648-12654.	1.2	14
241	Second Harmonic Generation and Hyperpolarizabilities of the Double-Cubane Compound [Sb₇S₈Br₂](AlCl₄)₃: Chalcogenide in Ionic Liquids. Journal of Physical Chemistry B, 2011, 115, 11763-11769.	1.2	14
242	Theoretical investigation for Li2CuSb as multifunctional materials: Electrode for high capacity rechargeable batteries and novel materials for second harmonic generation. Journal of Alloys and Compounds, 2011, 509, 7861-7869.	2.8	14
243	IR-induced features of AgGaGeS4 crystalline semiconductors. Journal of Physics and Chemistry of Solids, 2012, 73, 439-443.	1.9	14
244	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.	1.0	14
245	Influence of varying Germanium content on the optical function dispersion of Fe2MnSixGe1â^'x: An ab initio study. Journal of Magnetism and Magnetic Materials, 2013, 326, 210-216.	1.0	14
246	Photovoltaic characteristics of hybrid MEH-PPV-nanoparticles compound. Current Applied Physics, 2013, 13, 1894-1898.	1.1	14
247	Towards from indirect to direct band gap and optical properties of XYP2 (X=Zn, Cd; Y=Si, Ge, Sn). Physica B: Condensed Matter, 2014, 441, 94-99.	1.3	14
248	Structural and optical investigations of In doped ZnO binary compound. Materials Express, 2014, 4, 159-164.	0.2	14
249	Structural, elastic, thermal, electronic and optical properties of Ag2O under pressure. Computational Materials Science, 2014, 83, 474-480.	1.4	14
250	Electronic structure of GdX2 (X=Fe, Co and Ni) intermetallic compounds studied by the GGA+U method. Computational Materials Science, 2014, 87, 172-177.	1.4	14
251	Effect of lead and caesium on the mechanical, vibrational and thermodynamic properties of hexagonal fluorocarbonates: a comparative first principles study. RSC Advances, 2016, 6, 99885-99897.	1.7	14
252	Half metallicity and magnetism in graphene containing monovacancies decorated with Carbon/Nitrogen adatom. Journal of Alloys and Compounds, 2016, 663, 100-106.	2.8	14

#	Article	IF	Citations
253	Electronic structure and optical properties of dilute boron-bismide quaternary alloys B Ga1â€“As1â€“Bi /GaAs for infrared optoelectronic devices. Optik, 2017, 135, 57-69.	1.4	14
254	Electronic, bonding, linear, and nonlinear optical properties of Na2MGe2Q6 (M=Cd, Zn, Hg; Q=S, Se), Na2ZnSi2S6, and Na2ZnSn2S6 two metal-mixed chalcogenide compounds: Insights from an ab initio study. Journal of Physics and Chemistry of Solids, 2018, 119, 220-227.	1.9	14
255	Theoretical investigations of the electronic and optical properties of pure and alkali metal intercalated 1T-VSe2. Physica B: Condensed Matter, 2004, 349, 310-315.	1.3	13
256	Enhancement of the Kerr response in polymer-dispersed liquid crystal complexes due to incorporation of BiB3O6 nanocrystallites. Materials Letters, 2010, 64, 1176-1178.	1.3	13
257	Optoelectronic and transport properties of Zintl phase KBa2Cd2Sb3 compound. Computational Materials Science, 2014, 95, 328-336.	1.4	13
258	Linear and nonlinear optical properties of Î±-K2Hg3Ge2S8 and Î±-K2Hg3Sn2S8 compounds. Optical Materials, 2014, 37, 97-103.	1.7	13
259	Chairlike and Boatlike Graphane: Active Photocatalytic Water Splitting Solar-to-Hydrogen Energy Conversion under UV Irradiation. Journal of Physical Chemistry C, 2018, 122, 8076-8081.	1.5	13
260	Electron beam induced second-harmonic generation in Er3+ doped PbOâ€“GeO2 glasses containing silver nanoparticles. Journal of Materials Science: Materials in Electronics, 2009, 20, 87-91.	1.1	12
261	Elastic, electronic and optical properties of SiGe2N4 under pressure: An ab initio study. Physics Letters, Section A: General, Atomic and Solid State Physics, 2009, 373, 2393-2398.	0.9	12
262	Electro-optical properties of BixLayScz(BO3)4 (x+y+z=4) nanocrystallites having huntite structure incorporated into polymer matrices. Journal of Alloys and Compounds, 2009, 488, 291-293.	2.8	12
263	Role of tautomerism and solvatochromism in UVâ€“VIS spectra of arylhydrazones of Î²-diketones. Journal of Molecular Liquids, 2012, 171, 11-15.	2.3	12
264	Copper ion-exchanged channel waveguides optimization for optical trapping. Progress in Biophysics and Molecular Biology, 2013, 112, 118-123.	1.4	12
265	Linear and nonlinear optical susceptibilities of bilayer graphene. Materials Express, 2014, 4, 508-520.	0.2	12
266	Structural, electronic, and optical properties of orthorhombic and triclinic BiNbO4 determined via DFT calculations. Journal of Materials Science, 2014, 49, 7809-7818.	1.7	12
267	Electronic structure and transport properties of Ba2Cd2Pn3 (PnÂ=ÂAs and Sb): An efficient materials for energy conversion. Journal of Alloys and Compounds, 2016, 670, 1-11.	2.8	12
268	Lithium borate Li₃B₅O₈(OH)₂with large second harmonic generation and a high damage threshold in the deep-ultraviolet spectral range. Physical Chemistry Chemical Physics, 2017, 19, 30703-30714.	1.3	12
269	2D Hexagonal SnTe monolayer: a quasi direct band gap semiconductor with strain sensitive electronic and optical properties. European Physical Journal B, 2020, 93, 1.	0.6	12
270	A density functional study of second-order susceptibilities in calcium samarium oxyborate Ca₄SmO(BO₃)₃. Journal Physics D: Applied Physics, 2009, 42, 085406.	1.3	11

#	Article	IF	Citations
271	Laser induced microrelief superstructure of Ag/ITO seed-mediated nanocomposites. Superlattices and Microstructures, 2009, 46, 637-644.	1.4	11
272	Bandgap characters in GaAsâ€based ternary alloys. Crystal Research and Technology, 2010, 45, 59-69.	0.6	11
273	Density functional calculation for the first and second harmonic generation of the chalcopyrite Ga2AsSb. Computational Materials Science, 2011, 50, 886-892.	1.4	11
274	Crystallochemical affinity and optical functions of ZrGa2 and ZrGa3 compounds. Journal of Alloys and Compounds, 2013, 546, 14-19.	2.8	11
275	Electronic and optical properties of (Al x Ga1â^'x)1â^'y Mn y As single crystal: a new candidate for integrated optical isolators and spintronics. Journal of Materials Science, 2013, 48, 758-764.	1.7	11
276	Dispersion of the linear and nonlinear optical susceptibilities of Bismuth subcarbonate Bi2O2CO3: DFT calculations. Optical Materials, 2014, 38, 80-86.	1.7	11
277	Electronic structure, optical and thermoelectric transport properties of layered polyanionic hydrosulfate LiFeSO4OH: Electrode for Li-ion batteries. Journal of Alloys and Compounds, 2014, 591, 362-369.	2.8	11
278	Thermoelectric properties of the spin-polarized half-metallic ferromagnetic CsTe and RbSe compounds. RSC Advances, 2016, 6, 98197-98207.	1.7	11
279	Novel ternary semiconductor CdLa2X4 (X=S or Se) single crystal with efficient second harmonic generation in the visible spectral range. Journal of Alloys and Compounds, 2017, 728, 241-252.	2.8	11
280	Thermoelectric properties of TbFe2 and TbCo2 in C15- laves phase: Spin-polarized DFT+U approach. Journal of Magnetism and Magnetic Materials, 2017, 422, 287-298.	1.0	11
281	â€œTriggeringâ€•effect of second harmonic generation in centrosymmetric Î±-BaB2O4 crystals. Optical Materials, 2009, 31, 685-687.	1.7	10
282	Synthesis, IR, UVâ€“vis spectra, x-ray diffraction and band structure of a non-centrosymmetric borate single-crystal CaBiGaB₂O₇. Journal of Physics Condensed Matter, 2009, 21, 205402.	0.7	10
283	Comparative study on human and bovine AT-SC isolation methods. Progress in Biophysics and Molecular Biology, 2013, 113, 295-298.	1.4	10
284	Study of electronic structure, charge density, Fermi energy and optical properties of Cs2KTbCl6 and Cs2KEuCl6. Physica B: Condensed Matter, 2013, 431, 102-108.	1.3	10
285	First-principles calculations of the elastic, and electronic properties of YFe2, NiFe2 and YNiFe4 intermetallic compounds. Computational Materials Science, 2013, 73, 56-64.	1.4	10
286	Structural, elastic, thermal and electronic properties of M2X (MÂ=ÂSr, Ba and XÂ=ÂSi, Ge, Sn) compounds in anti-fluorite structure: first principle calculations. Indian Journal of Physics, 2015, 89, 369-375.	0.9	10
287	Transport properties of the n-type SrTiO₃/LaAlO₃ interface. RSC Advances, 2016, 6, 92887-92895.	1.7	10
288	Revealing the structural, elastic and thermodynamic properties of CdSexTe1â^'x (xÂ=Ââ€‹0, 0.25, 0.5, 0.75, 1). Journal of Alloys and Compounds, 2016, 667, 151-157.	2.8	10

#	Article	IF	Citations
289	Structure stability and magnetism in graphene impurity complexes with embedded V and Nb atoms. Journal of Magnetism and Magnetic Materials, 2017, 433, 109-115.	1.0	10
290	Photocatalytic water-splitting solar-to-hydrogen energy conversion: Novel LiMoO 3 (IO 3) molybdenyl iodate based on WO 3 -type sheets. Journal of Catalysis, 2017, 351, 1-9.	3.1	10
291	Photophysical, transport and structure properties of Tl10Hg3Cl16 single crystals: Novel photocatalytic water-splitting solar-to-hydrogen energy conversion. Journal of Catalysis, 2017, 352, 142-154.	3.1	10
292	Phase transition in BaThO3 from Pbnm to Ibmm turn the fundamental energy band gap from indirect to direct. Journal of Alloys and Compounds, 2019, 771, 607-613.	2.8	10
293	Computational investigation of structural, magnetic, elastic, and electronic properties of Half-Heusler ScVX (Xâ€‰=â€‰Si, Ge, Sn, and Pb) compounds. European Physical Journal Plus, 2021, 136, 1.	1.2	10
294	Thermoelectric, structural, electronic, magnetic, and thermodynamic properties of CaZn2Ge2 compound. European Physical Journal Plus, 2022, 137, 1.	1.2	10
295	Comparison of the Density of States Obtained from the X-ray Photoelectron Spectra with the Electronic Structure Calculations for Î±-BiB3O6. Japanese Journal of Applied Physics, 2009, 48, 011601.	0.8	9
296	Density Functional Calculation for Li2CuSn as an Electrode Material for Rechargeable Batteries. Journal of Physical Chemistry B, 2009, 113, 13208-13215.	1.2	9
297	Amino acid 2-aminopropanoic CH3CH(NH2)COOH crystals: materials for photo- and acoustoinduced optoelectronic applications. Journal of Materials Science: Materials in Electronics, 2012, 23, 1922-1931.	1.1	9
298	On the electronic nature of silicon and germanium based oxynitrides and their related mechanical, optical and vibrational properties as obtained from DFT and DFPT. Computational Materials Science, 2012, 53, 158-168.	1.4	9
299	Second harmonic generation imaging of the deep shade plant Selaginella erythropus using multifunctional twoâ€photon laser scanning microscopy. Journal of Microscopy, 2012, 248, 234-244.	0.8	9
300	Single-crystal oxoborate (Pb3O)2(BO3)2WO4: Growth and characterization. Materials Research Bulletin, 2012, 47, 2552-2560.	2.7	9
301	Erâ€“Pr doped tellurite glass nanocomposites for white light emitting diodes. Optics Communications, 2012, 285, 655-658.	1.0	9
302	Electronic and optical features of the mixed crystals Ag0.5Pb1.75Ge(S1â€“xSex)4. Journal of Materials Chemistry C, 2013, 1, 4667.	2.7	9
303	The influence of the lattice relaxation on the optical properties of GaNxAs1â^'x alloys. Solar Energy, 2013, 90, 134-143.	2.9	9
304	Electronic structure, optical and dielectric constant of compounds Indium-based: InAlP2, and InGaP2 in its chalcopyrite, CuPt and CuAu-I structures. Materials Science in Semiconductor Processing, 2013, 16, 1454-1465.	1.9	9
305	NaAuS chicken-wire-like semiconductor: Electronic structure and optical properties. Journal of Alloys and Compounds, 2014, 582, 6-11.	2.8	9
306	Density functional study of electronic, charge density, and chemical bonding properties of 9-methyl-3-Thiophen-2-Yl-Thieno [3,2-e] [1, 2, 4] Thriazolo [4,3-c] pyrimidine-8-Carboxylic acid ethyl ester crystals. Journal of Magnetism and Magnetic Materials, 2014, 361, 206-211.	1.0	9

#	Article	IF	Citations
307	Thermoelectric properties, electronic structure and optoelectronic properties of anisotropic Ba2Tl2CuO6 single crystal from DFT approach. Journal of Magnetism and Magnetic Materials, 2014, 354, 216-221.	1.0	9
308	Optoelectronic and thermoelectric properties of KAuX5 (XÂ=ÂS, Se): a first principles study. Journal of Materials Science, 2014, 49, 1179-1192.	1.7	9
309	Electronic structure, Fermi surface and optical properties of metallic compound Be8(B48)B2. Journal of Magnetism and Magnetic Materials, 2014, 351, 98-103.	1.0	9
310	Electronic and optical properties of the LiCdX (X = N, P, As and Sb) filled-tetrahedral compounds with the Tranâ€“Blaha modified Beckeâ€“Johnson density functional. Materials Research Bulletin, 2015, 64, 337-346.	2.7	9
311	First-principles calculation on dilute magnetic alloys in zinc blend crystal structure. Journal of Magnetism and Magnetic Materials, 2015, 385, 27-31.	1.0	9
312	Lead nitrate hydroxide: A strong second-order optical nonlinearity acentric crystal with high laser damage thresholds. Journal of Applied Physics, 2016, 119, .	1.1	9
313	Experimental and theoretical study of the electronic structure and optical spectral features of PbIn₆Te₁₀. RSC Advances, 2016, 6, 73107-73117.	1.7	9
314	Firstâ€principles calculations of structural, electronic, optical, and thermoelectric properties of ternary d â€metal sulfides <scp> Sc ₂ CdS ₄ </scp> and <scp> Y ₂ CdS ₄ </scp> compounds. International Journal of Energy Research, 2021, 45, 13657-13667.	2.2	9
315	Cationic variation for LnAl2Si2 (LnÂ=ÂY, Sm, Tb, Dy, Yb) compounds by density functional theory. Journal of Molecular Structure, 2022, 1252, 132136.	1.8	9
316	Structural, electronic and optical properties of SrCl2 under hydrostatic stress. European Physical Journal B, 2008, 61, 165-171.	0.6	8
317	Temperature anomalies of DEAâ€“CuCl4 and TEAâ€“CoCl2Br2/PMMA nanocomposites. Materials Letters, 2008, 62, 2084-2087.	1.3	8
318	Nonlinear absorption of fullerene- and nanotubes-doped liquid crystal systems. Physica E: Low-Dimensional Systems and Nanostructures, 2009, 41, 391-394.	1.3	8
319	UVâ€“vis absorption spectra of 1,4-dialkoxy-2,5-bis[2-(thien-2-yl)ethenyl]benzenes. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2009, 72, 394-398.	2.0	8
320	Band Structure, Density of States, and Optical Susceptibilities of a Novel Lithium Indium Orthoborate Li₃InB₂O₆. Journal of Physical Chemistry B, 2009, 113, 11583-11588.	1.2	8
321	X-ray Diffraction, X-ray Photoelectron Spectra, Crystal Structure, and Optical Properties of Centrosymmetric Strontium Borate Sr2B16O26. Journal of Physical Chemistry B, 2009, 113, 9161-9167.	1.2	8
322	Electronic band structure and optical properties of titanium oxyphosphates Li0.50Co0.25TiO(PO4) single crystals: An ab-initio calculations. Journal of Solid State Chemistry, 2011, 184, 2131-2138.	1.4	8
323	Optoelectronic properties of GaAs and AlAs under temperature effect. Optik, 2013, 124, 2128-2130.	1.4	8
324	Photothermal poling of glass complexes Ag2Sâ€“Ga2S3â€“P2S5. Optics Communications, 2013, 307, 1-4.	1.0	8

#	Article	IF	Citations
325	Dispersion of the linear and nonlinear optical susceptibilities of the CuAl(S1â^'xSex)2 mixed chalcopyrite compounds. Journal of Applied Physics, 2014, 116, .	1.1	8
326	Theoretical calculations for MUO3 (MÂ=ÂNa; K; Rb): DFTÂ+ÂU study. Journal of Organometallic Chemistry, 2014, 766, 22-33.	0.8	8
327	Nowotnyâ€"Juza NaZnX (X = P, As and Sb) as photovoltaic materials. Solar Energy, 2015, 115, 430-440.	2.9	8
328	From micro-to macroscopic: Understanding optical properties in zinc-blend-derived materials Cu2ZnYX4(XÂ=ÂS, Se, Te, YÂ=ÂSi, Ge, Sn) by means of the quantum chemical topology analysis. Journal of Alloys and Compounds, 2015, 653, 140-147.	2.8	8
329	Linear, nonlinear optical susceptibilities, hyperpolarizability, and space electronic charge density of meso silver(I) histidinate [Ag(D-his)]n (Hhis=histidine). Polyhedron, 2015, 85, 962-970.	1.0	8
330	DFT calculations for the electronic structure ofÂalpha phase of CsMgH3 as advanced hydrogenÂstorage materials. International Journal of Hydrogen Energy, 2016, 41, 2762-2770.	3.8	8
331	Effects of anion-ligands replacement on the Structural, Electronic and Magnetic properties of ThCo2X2 (XÂ=ÂSi, Ge). Chinese Journal of Physics, 2022, 77, 956-964.	2.0	8
332	Optical properties of alkaline-earth fluorohalides BaFX (X=Cl, Br, I) compounds. Solid-State Electronics, 2007, 51, 1133-1138.	0.8	7
333	Specific features of absorption and DSC for the DEA-CuCl4 nanoparticles incorporated into the PMMA polymer matrices. Physica B: Condensed Matter, 2008, 403, 2561-2566.	1.3	7
334	X-ray Diffraction, Crystal Structure, and Spectral Features of the Optical Susceptibilities of Single Crystals of the Ternary Borate Oxide Lead Bismuth Tetraoxide, PbBiBO₄. Journal of Physical Chemistry B, 2009, 113, 6640-6646.	1.2	7
335	Comparison of Bowing Behaviors Between IIIâ€"V and IIâ€"VI Common-Cation Semiconductor Ternary Alloys. Journal of Electronic Materials, 2010, 39, 178-186.	1.0	7
336	Photoinduced absorption and nonlinear optics of triglycine selenate single crystals under uniaxial pressure. Materials Letters, 2011, 65, 1734-1736.	1.3	7
337	Band structure, density of states, and crystal chemistry of ZrGa2 and ZrGa3 single crystals. Journal of Alloys and Compounds, 2013, 556, 259-265.	2.8	7
338	Electronic structure, density of electronic states, and the chemical bonding properties of 2,4-dihydroxyl hydrazone crystals (C13H11N3O4). Journal of Materials Science, 2013, 48, 3805-3811.	1.7	7
339	Transport properties of APdCu(Se₂)(Se₃) (A = K and Rb): new quaternary copper palladium polyselenides. RSC Advances, 2014, 4, 20102-20113.	1.7	7
340	Electronic structure and dispersion of optical function of tantalum nitride as a visible light photo-catalyst. Computational Materials Science, 2014, 89, 45-51.	1.4	7
341	Dispersion of the second harmonic generation in GaNxAs1â^'x (x=0.25, 0.5, 0.75) alloys. Journal of Alloys and Compounds, 2014, 589, 213-217.	2.8	7
342	Exploring and exploiting the influence of the compression mechanism on the transport properties of CrF3. RSC Advances, 2015, 5, 47569-47578.	1.7	7

#	Article	IF	Citations
343	Microcrystalline Î²-RbNd(MoO₄)₂: spin polarizing DFT+U. RSC Advances, 2015, 5, 44960-44968.	1.7	7
344	LiMoO 3 (IO 3), a novel molybdenyl iodate with strong second-order optical nonlinearity. Journal of Alloys and Compounds, 2016, 660, 32-38.	2.8	7
345	Novel dibenzothiophene chromophores with peripheral barbituric acceptors. Tetrahedron, 2019, 75, 130459.	1.0	7
346	Untangling electronic, optical and bonding properties of hexagonal bismuth borate SrBi2B2O7 crystal for ultraviolet opto-electronic applications: An ab initio study. Journal of Alloys and Compounds, 2019, 803, 1127-1135.	2.8	7
347	The effect of the phase transition on the optical properties of the lanthanum monopnictide compounds. Journal of Physics Condensed Matter, 2008, 20, 325207.	0.7	6
348	SYNTHESIS AND NLO PROPERTIES OF NEW CHROMOPHORES BASED ON IMIDAZO[1,2-A]PYRIDINE. Chemical Engineering Communications, 2009, 196, 1466-1474.	1.5	6
349	Laser treatment of seed-mediated nanostructured silver film morphology. Materials Chemistry and Physics, 2009, 113, 187-191.	2.0	6
350	High second harmonic generation signal from muscles and fascia pig's muscles using the twoâ€photon laser scanning microscope. Journal of Microscopy, 2009, 234, 280-286.	0.8	6
351	Enhancing the resolution of the forward second harmonic imaging using the two-photon laser scanning microscope. Micron, 2009, 40, 750-755.	1.1	6
352	Electrooptics parameters of the BiBO:Tm3+ glass nanoparticles embedded in polymer matrices. Journal of Materials Science: Materials in Electronics, 2010, 21, 726-729.	1.1	6
353	Density Functional Calculations, Electronic Structure, and Optical Properties of Molybdenum Bimetallic Nitrides Pt2Mo3N and Pd2Mo3N. Journal of Physical Chemistry B, 2011, 115, 3363-3370.	1.2	6
354	Structural, electronic, linear, and nonlinear optical properties of ZnCdTe₂ chalcopyrite. Physica Status Solidi (B): Basic Research, 2011, 248, 712-718.	0.7	6
355	An ab initio density functional study of the optical functions of 9-Methyl-3-Thiophen-2-YI-Thieno [3,2e] [1,2,4] Thriazolo [4,3c] Pyrimidine-8-Carboxylic Acid Ethyl Ester crystals. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2012, 95, 582-588.	2.0	6
356	Laser stimulated optical features of gold nanoparticles attached on ITO substrate. Physica E: Low-Dimensional Systems and Nanostructures, 2012, 44, 1182-1188.	1.3	6
357	Electronic structure and magneto-optic Kerr effect in ferromagnetic titanium oxyphosphates Li0.50Co0.25TiO(PO4): An ab-initio study. Journal of Alloys and Compounds, 2012, 527, 233-239.	2.8	6
358	Phase transition, electronic and optical properties of NaCl under pressure. Modern Physics Letters B, 2014, 28, 1450062.	1.0	6
359	Electronic band structure and optoelectronic properties of SrCu2X2 (XÂ=ÂAs, Sb): DFT calculation. Journal of Materials Science, 2014, 49, 5208-5217.	1.7	6
360	Thermoelectric properties of Li2PbGeS4 polar chalcopyrites single crystals as photovoltaic candidate. Computational Materials Science, 2014, 89, 52-56.	1.4	6

#	Article	IF	Citations
361	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.	1.9	6
362	Density of states, optical and thermoelectric properties of perovskite vanadium fluorides Na3VF6. Journal of Magnetism and Magnetic Materials, 2014, 358-359, 16-22.	1.0	6
363	Experimental and theoretical investigation of the electronic structure and optical properties of TlHgCl3 single crystal. Optical Materials, 2015, 47, 445-452.	1.7	6
364	Specific features of electronic structures and optical susceptibilities of g-BC₃ and t-BC₃ phases. Physical Chemistry Chemical Physics, 2015, 17, 8006-8016.	1.3	6
365	Revealing the origin of the strong second harmonic generation of Li2CdXS4 and Li2CdXS4 (Xâ€‰=â€‰Ge or) Tj ETQq1 1 0.784314	1.1	6
366	Full-potential calculations of the electronic and optical properties of 1T and 2H phases of TaS2 intercalated with lithium. Physica B: Condensed Matter, 2006, 373, 1-7.	1.3	5
367	Pockels effect in yttrium aluminum borate single crystals. Laser Physics, 2008, 18, 1204-1206.	0.6	5
368	X-ray photoelectron spectroscopy and full potential studies of the electronic density of state of ternary oxyborate Na3La9O3(BO3)8. Journal of Alloys and Compounds, 2009, 472, 30-34.	2.8	5
369	OPTICALLY-OPERATED ELASTOOPTICAL EFFECTS IN POLYMER MATRICES WITH NANOCRYSTALLITES. Functional Materials Letters, 2011, 04, 357-359.	0.7	5
370	Investigated stiffness of high performance superconductivity with nanoceria incorporated into polycrystalline magnesium diboride. Micro and Nano Letters, 2012, 7, 867.	0.6	5
371	Electronic structure, Fermi surface topology and spectroscopic optical properties of LaBaCo2O5.5 compound. Journal of Magnetism and Magnetic Materials, 2014, 363, 133-139.	1.0	5
372	INSULATOR TO METAL TRANSITION AND OPTICAL RESPONSE OF CsCl UNDER PRESSURE. International Journal of Modern Physics B, 2014, 28, 1450047.	1.0	5
373	Electrical transport properties of potassium germanide tungstates (K10Ge18WO4): A theoretical study. Solid State Sciences, 2014, 32, 26-34.	1.5	5
374	The influence of replacing Se by Te on electronic structure and optical properties of Tl4PbX3(X = Se or) Tj ETQq0 0 0 rgBT /Overlock 10	1.7	5
375	Specific features of the electronic structure and optical properties of skutterudites LaFe4X12 (X = P,) Tj ETQq1 1 0.784314 rgBT /Ove	1.7	5
376	AA- and ABA-stacked carbon nitride (C₃N₄): novel photocatalytic water splitting solar-to-hydrogen energy conversion. Physical Chemistry Chemical Physics, 2018, 20, 22972-22979.	1.3	5
377	First principles prediction of the elastic, electronic and optical properties of Sn3X4 (Xâ€¯=â€¯P, As, Sb, Bi) compounds: Potential photovoltaic absorbers. Chinese Journal of Physics, 2019, 59, 265-272.	2.0	5
378	First-principles calculations to investigate variation of cationic-ligand LmAl2Ge2 (Lmâ€‰=â€‰Ca, Y, La and Ce). Indian Journal of Physics, 2022, 96, 3151-3159.	0.9	5

#	Article	IF	Citations
379	Optical properties of some laves phases compounds. Current Opinion in Solid State and Materials Science, 2008, 12, 39-43.	5.6	4
380	Electronic band structures of AV2(A = Ta, Ti, Hf and Nb) Laves phase compounds. Journal of Physics Condensed Matter, 2009, 21, 025502.	0.7	4
381	Laser stimulated bistability in the Yb doped Nd gallate. Materials Letters, 2009, 63, 1410-1412.	1.3	4
382	Existence or absence of bandgap bowing in II-VI ternary alloys: Comparison between common-anion and common-cation cases. Journal of Physics: Conference Series, 2010, 209, 012024.	0.3	4
383	Laser induced effects in PbOâ€“Bi2O3â€“Ga2O3â€“BaO: Eu glasses. Optics Communications, 2010, 283, 3049-3051.	1.0	4
384	Laser operated elasto-optical features of La2CaB10O19:Pr3+ polymer nanocomposites. Journal of Luminescence, 2012, 132, 2577-2580.	1.5	4
385	Linear optical susceptibilities of the oxoborate (Pb3O)2(BO3)2WO4: theory and experiment. Journal of Materials Science, 2012, 47, 5794-5800.	1.7	4
386	DFT calculation of the electronic structure and optical properties of two strontium germanium nitrides: Î±-Sr2GeN2 and Î²-Sr2GeN2. Journal of Alloys and Compounds, 2013, 559, 181-187.	2.8	4
387	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.	1.0	4
388	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.	1.0	4
389	Theoretical investigation of some specific features of the electronic structure and optical properties of Benzoic Acid 2-Amino-4,6-Dimethylpyrimidine (1:1) co-crystals. Optical Materials, 2015, 46, 216-222.	1.7	4
390	Effect of X on the transport properties of skutterudites LaFe 4 X 12 (XÂ=ÂP, As and Sb) compounds. Journal of Alloys and Compounds, 2015, 651, 176-183.	2.8	4
391	Characterization of multiferroic Bi0.8RE0.2FeO3 powders (RE=Nd3+, Eu3+) grown by the solâ€“gel method. Materials Letters, 2015, 139, 104-107.	1.3	4
392	Thermoelectric and optoelectronic properties of a heterocyclic isoxazolone nucleus compound. Materials Science in Semiconductor Processing, 2015, 30, 197-207.	1.9	4
393	Spin-polarization in filled-skutterudites LaFe 4 Pn 12 (Pn =P, As and Sb). Journal of Magnetism and Magnetic Materials, 2016, 401, 684-694.	1.0	4
394	Electronic structure and optical properties of Î²-RbSm(MoO 4) 2 from spin polarization calculations: DFT+U. Materials Chemistry and Physics, 2017, 192, 260-267.	2.0	4
395	Structural, electronic and thermoelectric properties of topological semimetal lanthanum monopnicitide LaBi. Physics Letters, Section A: General, Atomic and Solid State Physics, 2020, 384, 126789.	0.9	4
396	Structural, electronic and optoelectronic properties of <scp> AB ₅ C ₈ </scp> (<scp>A = Cu/Ag; B = In and C = S, Se and Te</scp>) compounds. International Journal of Energy Research, 2021, 45, 4014-4025.	2.2	4

#	Article	IF	Citations
397	Specific Features of Li₅La₃M₂O₁₂ (M = Nb, Ta) Single Crystals: Electrolyte for Solid States Batteries. Science of Advanced Materials, 2014, 6, 1716-1726.	0.1	4
398	Laser operated borate polymer nanocomposites. Journal of Alloys and Compounds, 2011, 509, 1271-1274.	2.8	3
399	Theoretical investigation of the elastic, thermodynamic, electronic and magnetic properties of PrNi2Si2 and PrNi2Ge2. Computational Materials Science, 2012, 54, 303-311.	1.4	3
400	A density functional study of the electronic properties of bismuth subcarbonate Bi2O2CO3. Solid State Sciences, 2014, 38, 138-142.	1.5	3
401	Thermoelectric, electronic, optical and chemical bonding properties of Ba2PrRuO6: At temperature 7 K and 150 K. Materials Research Bulletin, 2015, 61, 551-559.	2.7	3
402	Single Brillouin frequency shifted S-band multi-wavelength Brillouin-Raman fiber laser utilizing fiber Bragg grating and Raman amplifier in ring cavity. Optical Materials, 2016, 60, 38-44.	1.7	3
403	Electronic structure, first and second order physical properties of MPS4: a theoretical study. Materials Science-Poland, 2016, 34, 275-285.	0.4	3
404	Evanescent field optimization on Y-branch silicon nitride optical waveguide for biosensing. Materials Letters, 2016, 173, 127-130.	1.3	3
405	Influence of an oxygen vacancy on the electronic structure of the asymmetric mixed borateâ€“carbonate Pb₇O(OH)₃(CO₃)₃(BO₃). RSC Advances, 2016, 6, 18965-18972.	1.7	3
406	Structural and electronic properties of InN_xP_{1-x}alloy in full range (0 â‰¤ x â‰¤1). Philosophical Magazine, 2016, 96, 991-1005.	0.7	3
407	Formation of metastable phases of ferrous sulfide via pulsed Nd:YAG laser deposition: Experimental and theoretical study. Journal of Alloys and Compounds, 2017, 723, 689-697.	2.8	3
408	Effect of Si and Ge Surface Doping on the Be2C Monolayer: Case Study on Electrical and Optical Properties. Silicon, 2018, 10, 1893-1902.	1.8	3
409	One- and two-dimensional search of an equation of state using a newly released 2DRoptimize package. Journal of Physics and Chemistry of Solids, 2018, 116, 131-136.	1.9	3
410	Bismuth-containing semiconductors GaAs1â^'xBix for energy conversion: Thermoelectric properties. Materials Science in Semiconductor Processing, 2022, 148, 106850.	1.9	3
411	Acoustically induced light gyration in nickel nanoparticles. Optics and Laser Technology, 2008, 40, 499-504.	2.2	2
412	Nonlinear optical study of amorphous SiN:H films on the Si(111) substrate. Laser Physics, 2008, 18, 999-1002.	0.6	2
413	Photoinduced piezooptical changes caused by microsecond CO2 Infrared lasers in lead-germanate rare earth tridoped glasses. Materials Letters, 2011, 65, 1445-1447.	1.3	2
414	Specific features of electronic structures and nonlinear optical susceptibilities of superhard metallic diamond-like t-B2CN compound. RSC Advances, 2014, 4, 64947-64955.	1.7	2

#	Article	IF	Citations
415	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.	1.1	2
416	Towards a deeper understanding of physical and chemical properties of Ag2Hgâ–¡I4 and Cu2Hgâ–¡I4 defective crystals, from first principles calculations. Materials Science in Semiconductor Processing, 2014, 27, 433-445.	1.9	2
417	Glass formation and the third harmonic generation of Cu2Seâ€“GeSe2â€“As2Se3 glasses. Journal of Applied Physics, 2014, 116, 143102.	1.1	2
418	Dispersion of electronic bands in intermetallic compound LiBe and related properties. Indian Journal of Physics, 2015, 89, 1051-1058.	0.9	2
419	The influence of replacing the pnicogens As by Sb on the optical properties of the Zintl phases Ba2Cd2Pn3 (PnÂ=ÂAs and Sb). Journal of Alloys and Compounds, 2015, 648, 1-6.	2.8	2
420	Non-centrosymmetric LiBaB9O15 single crystal: growth and characterization. Indian Journal of Physics, 2015, 89, 923-929.	0.9	2
421	First principles treatment of structural, optical, and thermoelectric properties of Li7MnN4 as electrode for a Li secondary battery. Materials Research Bulletin, 2015, 61, 306-314.	2.7	2
422	Revealing the spin-polarized optical properties of monoclinic Î±-Eu2(MoO4)3: a DFT + U approach. RSC Advances, 2016, 6, 51675-51682.	1.7	2
423	Investigation of structural, electronic, and optical properties of the monoclinic and triclinic polymorphs of hexamethylenetetraminium 2,4-dinitrophenolate monohydrate <mml:math altimg="si1.gif" overflow="scroll" xmlns:xocs="http://www.elsevier.com/xml/xocs/dtd" xmlns:xs="http://www.w3.org/2001/XMLSchema" xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance" xmlns="http://www.elsevier.com/xml/ja/dtd" xmlns:ja="http://www.elsevier.com/xml/ja/dtd" xmlns:mml="http://www.w3.org/1998/Math/MathML"	2.0	2
424	Revealing the influence of the compression mechanism on the electronic structure and the related properties of CrF 3. Journal of Alloys and Compounds, 2016, 660, 1-10.	2.8	2
425	Electronic, bonding and optical properties of the LiGaGe2X6 (Xâ€¯=â€¯S, Se, and Te) compounds: An ab initio study. Optik, 2019, 180, 782-791.	1.4	2
426	Phase Transition as an Emergent Phenomenon Analysed by Violation of Structural Invariant (M, BM). Mendel, 2020, 26, 45-50.	0.5	2
427	Reduction of the pulse duration of the ultrafast laser pulses of the Two-Photon Laser Scanning Microscopy (2PLSM). BMC Research Notes, 2008, 1, 39.	0.6	1
428	ELECTRONEGATIVITY EFFECTS ON THE BANDGAP BOWING CHARACTERS IN COMPOUND-SEMICONDUCTOR TERNARY ALLOYS. International Journal of Nanoscience, 2010, 09, 609-617.	0.4	1
429	Specific features of electronic structure and linear optical properties of some pseudocubic compounds. Computational Materials Science, 2010, 48, 326-335.	1.4	1
430	Influence of different exchange correlation potentials on band structure and optical constant calculations of ZrGa2 and ZrGe2 single crystals. Computational Materials Science, 2013, 78, 134-139.	1.4	1
431	Bicolor laser stimulated elastooptical effect in the 2-cyclooctylamino-5-nitropyridine-C70 system. Journal of Materials Science: Materials in Electronics, 2013, 24, 1875-1877.	1.1	1
432	Magnetic and thermoelectric properties of three different atomic ratio of Bi/Mn in BiMn2O5: DFT approach. Journal of Magnetism and Magnetic Materials, 2014, 369, 234-242.	1.0	1

#	Article	IF	Citations
433	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.	1.9	1
434	First principle investigation of electronic structure and optical behaviors of 2-amino-4-fluorododec-4-encarbolic acid. Materials Science in Semiconductor Processing, 2015, 31, 302-309.	1.9	1
435	Electronic structure of alkali-metal/alkaline-earth-metal fluorine beryllium borate NaSr3Be3B3O9F4 single crystal: DFT approach. Optical Materials, 2015, 48, 25-30.	1.7	1
436	Second harmonic generation from the novel polar polymorph Î±/Î²-BaTeMo₂O₉ phases. RSC Advances, 2015, 5, 70992-71001.	1.7	1
437	The electronic band structure of polar polymorph Î±/Î²-BaTeMo 2 O 9 phases. Journal of Alloys and Compounds, 2015, 651, 308-315.	2.8	1
438	Electronic properties of orthorhombic BaSn2S5 single crystal. Indian Journal of Physics, 2015, 89, 437-443.	0.9	1
439	Electronic and optical properties of Î²â€²-Tb2(MoO4)3: DFT+U approach. European Physical Journal B, 2016, 89, 1.	0.6	1
440	Exploring the electronic structure of Pb 2+ ions containing material Pb 16 (OH) 16 (NO 3) 16. Journal of Physics and Chemistry of Solids, 2016, 99, 75-81.	1.9	1
441	Revealing the electronic structure and optical properties of K₆[Mo₄O₈F₁₀] novel molybdenum oxyfluoride materials. Philosophical Magazine, 2016, 96, 3131-3142.	0.7	1
442	Realization and computational analysis of splitting in higher order optical vortices. Optik, 2016, 127, 5757-5760.	1.4	1
443	Spin-polarized antiferromagnetic CaCoSO single crystal: First-principles study. Journal of Alloys and Compounds, 2017, 711, 229-234.	2.8	1
444	CaCoSO diluted magnetic antiferromagnet semiconductor as efficient thermoelectric materials. Materials Research Bulletin, 2017, 94, 22-30.	2.7	1
445	Optical features of novel semiconducting crystals Tl1â€“xGa1â€“xSnxSe2 (x=0.05; 0.1). Optik, 2020, 206, 163572.	1.4	1
446	Laser-stimulated Pockels effect in CdBr2/Cu polymer nanocomposites. Physica E: Low-Dimensional Systems and Nanostructures, 2020, 118, 113904.	1.3	1
447	Second harmonic generation signal from deep shade moisture plants USING the two-photon laser scanning microscope. , 2009, , .		0
448	Temperature dependences of the second order susceptibilities in the novel borate LiCsB<inf>4</inf>O<inf>7</inf> single crystal. , 2009, , .		0
449	DFT calculation of the electronic and optical properties of Ag2PdO2 from X-ray and neutron crystallographic data. Solid State Sciences, 2013, 22, 50-55.	1.5	0
450	Motion behavior of mammalian AT-SC under evanescent field illumination. , 2015, , .		0

#	Article	IF	Citations
451	Theoretical study of the new zintl phases compounds K2ACdSb2 (A=(Sr, Ba)). Physica B: Condensed Matter, 2015, 464, 9-16.	1.3	0
452	Mixed alkali and alkaline-earth borate Li2Sr4B12O23 single crystal. Optical Materials, 2015, 48, 165-171.	1.7	0
453	Critical analysis on degradation mechanism of dye-sensitized solar cells. , 2015, , .		0
454	Thermoelectric Properties of the Intermetallic Quasi-Two-Dimensional Layered Structure LiBe. Journal of Electronic Materials, 2016, 45, 5546-5553.	1.0	0
455	Revealing the transport properties of the spin-polarized Î²â€²-Tb 2 (MoO 4) 3 : DFT+U. Journal of Magnetism and Magnetic Materials, 2017, 441, 124-130.	1.0	0
456	Metal Hydrides: Electronic Band Structureâ˜†. , 2017, , .		0
457	Modeling Complex Systems by Structural Invariants Approach. Complexity, 2021, 2021, 1-17.	0.9	0
458	Enhancement in magnetic parameters of L10-FeNi on Pd-substitution for permanent magnets. Indian Journal of Physics, 0, , 1.	0.9	0
459	Second Harmonic Generation Signal from Biological Materials Using Multi-Functional Two-Photon Laser Scanning Microscopy. , 0, , .		0