Sushil Auluck

List of Publications by Year
in descending order

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307	7,204	66343	102487
papers	citations	42 h-index	66 g-index

323	323	323	6639
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	High Thermoelectric Performance in n-Type Degenerate ZrNiSn-Based Half-Heusler Alloys Driven by Enhanced Weighted Mobility and Lattice Anharmonicity. ACS Applied Energy Materials, 2021, 4, 3393-3403.	5.1	30
2	Enhanced thermoelectric performance of Bi0.5Sb1.5Te3 via Ni-doping: A Shift of peak ZT at elevated temperature via suppressing intrinsic excitation. Journal of Materiomics, 2021, 7, 1264-1274.	5.7	9
3	Coupling ferroelectric polarization and anisotropic charge migration for enhanced CO2 photoreduction. Applied Catalysis B: Environmental, 2021, 284, 119709.	20.2	74
4	Enhancing gas adsorption properties of borophene by embedding transition metals. Computational Condensed Matter, 2020, 22, e00436.	2.1	18
5	Influence of defect pairs in Ga-based ordered defect compounds: a hybrid density functional study. Canadian Journal of Physics, 2020, 98, 770-777.	1.1	0
6	Band Structure Modification and Mass Fluctuation Effects of Isoelectronic Germanium-Doping on Thermoelectric Properties of ZrNiSn. ACS Applied Energy Materials, 2020, 3, 1349-1357.	5.1	27
7	Strain induced optoelectronic properties of two dimensional MnPSe₃/WS₂ heterostructure. Journal of Physics Condensed Matter, 2020, 32, 315501.	1.8	4
8	Optimization of electrical and thermal transport properties of Fe0.25Co0.75Sb3 Skutterudite employing the isoelectronic Bi-doping. Intermetallics, 2020, 123, 106796.	3.9	10
9	Enhancement in thermoelectric performance of single step synthesized Mg doped Cu2Se: An experimental and theoretical study. Intermetallics, 2019, 112, 106541.	3.9	29
10	Collective Effect of Fe and Se To Improve the Thermoelectric Performance of Unfilled p-Type CoSb₃ Skutterudites. ACS Applied Energy Materials, 2019, 2, 1067-1076.	5.1	32
11	Spin-dependent scattering induced negative magnetoresistance in topological insulator Bi2Te3 nanowires. Scientific Reports, 2019, 9, 7836.	3.3	16
12	Theoretical characterization of C doped SiGe monolayer. Journal of Applied Physics, 2019, 125, 145703.	2.5	4
13	Tin doped Cu3SbSe4: A stable thermoelectric analogue for the mid-temperature applications. Materials Research Bulletin, 2019, 113, 38-44.	5.2	15
14	Ferroelectric polarization promoted bulk charge separation for highly efficient CO2 photoreduction of SrBi4Ti4O15. Nano Energy, 2019, 56, 840-850.	16.0	144
15	Magnetism by embedding 3d transition metal atoms into germanene. Journal Physics D: Applied Physics, 2018, 51, 225006.	2.8	6
16	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.	3.1	60
17	Cation modified A 2 (Ba, Sr and Ca) ZnWO 6 cubic double perovskites: A theoretical study. Computational Condensed Matter, 2018, 14, 27-35.	2.1	19
18	Electronic structure, defect properties, and hydrogen storage capacity of 2H-WS2: A first-principles study. International Journal of Hydrogen Energy, 2018, 43, 23126-23134.	7.1	12

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19	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.	4.0	21
20	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.	6.1	33
21	Mono and bi-layer germanene as prospective anode material for Li-ion batteries: A first-principles study. Computational Condensed Matter, 2018, 16, e00314.	2.1	25
22	Unexplored photoluminescence from bulk and mechanically exfoliated few layers of Bi2Te3. Scientific Reports, 2018, 8, 9205.	3.3	15
23	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.	3.6	31
24	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.	6.2	10
25	Oxygen Induced Enhanced Photoanodic Response of ZnTe:O Thin Films: Modifications in Optical and Electronic Properties. Journal of Physical Chemistry C, 2017, 121, 1488-1497.	3.1	8
26	Role of spinâ€“orbit interaction on the nonlinear optical response of CsPbCO₃F using DFT. Physical Chemistry Chemical Physics, 2017, 19, 31255-31266.	2.8	22
27	Thermal conductivity of thermoelectric material Î²-Cu2Se: Implications on phonon thermal transport. Applied Physics Letters, 2017, 111, .	3.3	9
28	An interaction potential to study the thermal structure evolution of a thermoelectric material: Î²â€Cu₂Se. Journal of Computational Chemistry, 2017, 38, 2161-2170.	3.3	20
29	Band Gap Tuning Of ZnO 1-3x N 2x F x Alloys: A First Principles Study. Materials Today: Proceedings, 2017, 4, 5700-5705.	1.8	1
30	Two haloid borate crystals with large nonlinear optical response. Physical Chemistry Chemical Physics, 2017, 19, 18416-18425.	2.8	23
31	Theoretical insights into kesterite and stannite phases of Cu2(Sn1â€“XGeX)ZnSe4 based alloys: A prospective photovoltaic material. AIP Advances, 2016, 6, 125303.	1.3	5
32	Stability, electronic, and optical properties of wurtzite Cu2CdxZn1â^'xSnS4 alloys as photovoltaic materials: First-principles insight. Physical Review B, 2016, 94, .	3.2	9
33	Band gap engineering of CuAl_{1â^'x}In_xS₂alloys for photovoltaic applications: a first principles study. Journal Physics D: Applied Physics, 2016, 49, 205103.	2.8	4
34	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.	3.6	14
35	Experimental and theoretical study of the electronic structure and optical spectral features of PbIn₆Te₁₀. RSC Advances, 2016, 6, 73107-73117.	3.6	9
36	Band gap engineering of ZnO substituted with nitrogen and fluorine, ZnO_{1â^'3x}N_{2x}F_x: a hybrid density functional study. RSC Advances, 2016, 6, 99088-99095.	3.6	5

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37	Mg9Si5: a potential non-toxic thermoelectric material for mid-temperature applications. RSC Advances, 2016, 6, 62445-62450.	3.6	6
38	Luminescence and advanced mass spectroscopic characterization of sodium zinc orthophosphate phosphor for lowâ€cost lightâ€emitting diodes. Luminescence, 2016, 31, 348-355.	2.9	4
39	LiMoO 3 (IO 3), a novel molybdenyl iodate with strong second-order optical nonlinearity. Journal of Alloys and Compounds, 2016, 660, 32-38.	5.5	7
40	Electrical transport and mechanical properties of thermoelectric tin selenide. RSC Advances, 2016, 6, 11562-11569.	3.6	44
41	A DFT study of the electronic and optical properties of a photovoltaic absorber material Cu2ZnGeS4 using GGA and mBJ exchange correlation potentials. Journal of Alloys and Compounds, 2016, 675, 236-243.	5.5	22
42	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.	3.6	3
43	Experimental and theoretical investigation of the electronic structure and optical properties of TlHgCl3 single crystal. Optical Materials, 2015, 47, 445-452.	3.6	6
44	Thermodynamical and electronic properties of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si0009.gif" overflow="scroll"><mml:mrow><mml:msub><mml:mrow><mml:mi mathvariant="normal">B</mml:mi></mml:mrow><mml:mrow><mml:mi>x</mml:mi></mml:mrow></mml:msub></mml:mrow><mml:mr mathvariant="normal">N</mml:mi></mml:math>alloys: A first principle. Journal of Physics and Chemistry of Solids, 2015, 86, 101-107.	4.0	16
45	Electronic structure of alkali-metal/alkaline-earth-metal fluorine beryllium borate NaSr3Be3B3O9F4 single crystal: DFT approach. Optical Materials, 2015, 48, 25-30.	3.6	1
46	Anisotropy and high thermopower of LaOBiS2. Journal of Alloys and Compounds, 2015, 626, 208-211.	5.5	9
47	Non-centrosymmetric LiBaB9O15 single crystal: growth and characterization. Indian Journal of Physics, 2015, 89, 923-929.	1.8	2
48	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.	2.8	64
49	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.	2.5	32
50	Band gap engineering of Si-Ge alloys for mid-temperature thermoelectric applications. AIP Advances, 2015, 5, 037145.	1.3	9
51	An ab-initio study of CuInSe2 based ordered defect compounds. Materials Chemistry and Physics, 2015, 162, 372-379.	4.0	0
52	Thermoelectric properties of Nowotnyâ€“Juza NaZnX (X = P, As and Sb) compounds. Computational Materials Science, 2015, 96, 90-95.	3.0	46
53	Linear and nonlinear optical susceptibilities of bilayer graphene. Materials Express, 2014, 4, 508-520.	0.5	12
54	Band structure and transport studies of copper selenide: An efficient thermoelectric material. Applied Physics Letters, 2014, 105, .	3.3	34

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55	Optical anisotropy in bismuth titanate: An experimental and theoretical study. Journal of Applied Physics, 2014, 115, 133509.	2.5	3
56	Adsorbing H2S onto a single graphene sheet: A possible gas sensor. Journal of Applied Physics, 2014, 116, .	2.5	36
57	Dispersion of the linear and nonlinear optical susceptibilities of Bismuth subcarbonate Bi2O2CO3: DFT calculations. Optical Materials, 2014, 38, 80-86.	3.6	11
58	Dispersion of the linear and nonlinear optical susceptibilities of the CuAl(S1â˜'xSex)2 mixed chaclcopyrite compounds. Journal of Applied Physics, 2014, 116, .	2.5	8
59	Density functional study of electronic, charge density, and chemical bonding properties of 9-methyl-3-Thiophen-2-YI-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.	2.3	9
60	Effects of inter-site chemical disorder on the magnetic properties of MnBi. Journal of Magnetism and Magnetic Materials, 2014, 363, 18-20.	2.3	11
61	Electronic band structure and specific features of AA- and AB-stacking of carbon nitride (C3N4): DFT calculation. RSC Advances, 2014, 4, 6957.	3.6	32
62	Thermoelectric properties of a single graphene sheet and its derivatives. Journal of Materials Chemistry C, 2014, 2, 2346.	5.5	79
63	A density functional study of the electronic properties of bismuth subcarbonate Bi2O2CO3. Solid State Sciences, 2014, 38, 138-142.	3.2	3
64	Linear and nonlinear optical properties for AA and AB stacking of carbon nitride polymorph (C₃N₄). RSC Advances, 2014, 4, 11967-11974.	3.6	30
65	Thermoelectric properties of Cu3SbSe3 with intrinsically ultralow lattice thermal conductivity. Journal of Materials Chemistry A, 2014, 2, 15829-15835.	10.3	47
66	Electronic and optical properties of chair-like and boat-like graphane. RSC Advances, 2014, 4, 37411-37418.	3.6	25
67	Study of ferromagnetic instability in -MnAl, using first-principles. Journal of Alloys and Compounds, 2014, 601, 234-237.	5.5	18
68	An insight into evolution of electronic, magnetic, optical, and vibrational properties of ultrathin Pd nanowires. Journal of Nanoparticle Research, 2013, 15, 1.	1.9	4
69	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.	3.0	1
70	Electronic and optical features of the mixed crystals Ag0.5Pb1.75Ge(S1â€"xSex)4. Journal of Materials Chemistry C, 2013, 1, 4667.	5.5	9
71	Room Temperature Nanoscale Ferroelectricity in MagnetoelectricGaFeO3Epitaxial Thin Films. Physical Review Letters, 2013, 111, 087601.	7.8	99
72	Optical Spectra and Band Structure of Ag_xGa_xGe_{1â€"x}Se₂ (x = 0.333,) TjETQq0 0 0 rgBT /Ov 15220-15231.	2.6	36

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73	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.	2.8	150
74	Crystallochemical affinity and optical functions of ZrGa2 and ZrGa3 compounds. Journal of Alloys and Compounds, 2013, 546, 14-19.	5.5	11
75	Magnetic CrX and MnX (X=Si, Ge, and As) nanowires: Stability enhancement and linearization. Journal of Alloys and Compounds, 2013, 547, 138-146.	5.5	2
76	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.	3.7	20
77	Dispersion of the linear and nonlinear optical susceptibilities of disilver germanium sulfide from DFT calculations. Journal of Materials Science, 2013, 48, 1955-1965.	3.7	21
78	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.	2.6	38
79	Band structure, density of states, and crystal chemistry of ZrGa2 and ZrGa3 single crystals. Journal of Alloys and Compounds, 2013, 556, 259-265.	5.5	7
80	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.	3.7	7
81	Engineering polarization rotation in ferroelectric bismuth titanate. Applied Physics Letters, 2013, 102, .	3.3	12
82	Electronic structure, charge density, and chemical bonding properties of C11H8N2O o-methoxydicyanovinylbenzene (DIVA) single crystal. Journal of Materials Science, 2013, 48, 5157-5162.	3.7	20
83	Mg3Sb2-based Zintl compound: a non-toxic, inexpensive and abundant thermoelectric material for power generation. RSC Advances, 2013, 3, 8504.	3.6	133
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.	2.6	39
85	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.	0.7	46
86	Photoconducting state and its perturbation by electrostatic fields in oxide-based two-dimensional electron gas. Physical Review B, 2012, 86, .	3.2	46
87	Electronic and vibrational properties of vanadium-carbide nanowires. Journal of Applied Physics, 2012, 112, .	2.5	3
88	Electronic and optical properties of free-standing and supported vanadium nanowires. Journal of Applied Physics, 2012, 111, 093506.	2.5	8
89	Evolution of ferromagnetic and spin-wave resonances with crystalline order in thin films of full-Heusler alloy Co2MnSi. Journal of Applied Physics, 2012, 111, 023912.	2.5	28
90	Effect of site-disorder on magnetism and magneto-structural coupling in gallium ferrite: A first-principles study. Journal of Applied Physics, 2012, 111, .	2.5	16

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91	Linear and nonlinear optical susceptibilities and hyperpolarizability of borate LiNaB4O7 single crystals: Theory and experiment. Journal of Applied Physics, 2012, 112, .	2.5	20
92	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.	2.2	9
93	Dispersion of Linear, Nonlinear Optical Susceptibilities and Hyperpolarizability of C₁₁H₈N₂O (o-Methoxydicyanovinylbenzene) Crystals. Journal of Physical Chemistry B, 2012, 116, 13338-13343.	2.6	31
94	Implications of nanostructuring on the thermoelectric properties in half-Heusler alloys. Applied Physics Letters, 2012, 101, .	3.3	37
95	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.	3.9	6
96	Ab initio study of magnetism in FeSe and FeTe. , 2012, , .		3
97	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.	5.5	6
98	Effect of pressure on itinerant magnetism and spin disorder in cubic FeGe. Journal of Physics Condensed Matter, 2012, 24, 096003.	1.8	8
99	Structural, electronic properties and charge density distribution of the LiNaB4O7: Theory and experiment. Materials Chemistry and Physics, 2012, 137, 346-352.	4.0	16
100	Single-crystal oxoborate (Pb3O)2(BO3)2WO4: Growth and characterization. Materials Research Bulletin, 2012, 47, 2552-2560.	5.2	9
101	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.	2.6	43
102	Doping and temperature dependence of thermoelectric properties in Mg2(Si,Sn). Physical Review B, 2012, 86, .	3.2	126
103	Effects of site disorder, off-stoichiometry and epitaxial strain on the optical properties of magnetoelectric gallium ferrite. Journal of Physics Condensed Matter, 2012, 24, 435501.	1.8	14
104	Chalcogen height dependence of magnetism and Fermiology in FeTe_xSe_{1â^'x}. Superconductor Science and Technology, 2012, 25, 095002.	3.5	18
105	Linear optical susceptibilities of the oxoborate (Pb3O)2(BO3)2WO4: theory and experiment. Journal of Materials Science, 2012, 47, 5794-5800.	3.7	4
106	Absorption and photoconductivity spectra of Ag2GeS3 crystal: Experiment and theory. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2012, 93, 274-279.	3.9	25
107	Bismuth in gallium arsenide: Structural and electronic properties of GaAs1â^'xBix alloys. Journal of Solid State Chemistry, 2012, 186, 47-53.	2.9	27
108	Energetics and electronic structure of La/Sr disorder at the interface of SrTiO₃/LaTiO₃ heterostructure. Applied Physics Letters, 2011, 99, 081915.	3.3	4

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109	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.	2.6	14
110	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.	2.6	52
111	Normal state and superconducting properties of Rh₁₇S₁₅and Pd₁₇Se₁₅. Superconductor Science and Technology, 2011, 24, 105015.	3.5	11
112	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.	2.8	155
113	Electronic structure, chemical bonding features, and electron charge density of the double-cubane single crystal [Sb7S8Br2](AlCl4)3. Applied Physics Letters, 2011, 98, 201903.	3.3	15
114	Density Functional Calculations, Electronic Structure, and Optical Properties of Molybdenum Bimetallic Nitrides Pt2Mo3N and Pd2Mo3N. Journal of Physical Chemistry B, 2011, 115, 3363-3370.	2.6	6
115	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.	5.5	47
116	Bismuth-containing semiconductors: Linear and nonlinear optical susceptibilities of GaAs1â^'xBix alloys. Journal of Alloys and Compounds, 2011, 509, 9685-9691.	5.5	33
117	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
118	Photo-absorption spectra of small hydrogenated silicon clusters using the time-dependent density functional theory. Journal of Physics and Chemistry of Solids, 2011, 72, 1096-1100.	4.0	10
119	Electronic and optical properties of rare earth trifluorides RF3 (R=La, Ce, Pr, Nd, Gd and Dy). Materials Chemistry and Physics, 2011, 129, 349-355.	4.0	12
120	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.	4.0	16
121	First-principles comparison of the cubic and tetragonal phases of. Chemical Physics Letters, 2011, 504, 148-152.	2.6	3
122	Structural, thermodynamic and optical properties of MgF2 studied from first-principles theory. Journal of Solid State Chemistry, 2011, 184, 343-350.	2.9	75
123	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.	2.9	8
124	Electronic and optical properties of high pressure stable phases of ZnS: Comparison of FPLAPW and PW-PP results. Optics Communications, 2011, 284, 20-26.	2.1	10
125	Electronic structure, Born effective charges and spontaneous polarization in magnetoelectric gallium ferrite. Journal of Physics Condensed Matter, 2011, 23, 325902.	1.8	39
126	Physical property and electronic structure characterization of bulk superconducting Bi₃Ni. Superconductor Science and Technology, 2011, 24, 085002.	3.5	42

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127	Theoretical studies on electronic and magnetic properties of ultrathin Mo nanowires. Journal of Applied Physics, 2010, 107, 024307.	2.5	3
128	Optical and magneto-optical properties of Fe4â^'xCox (x = 1â€“3). European Physical Journal B, 2010, 73, 423-432.	1.5	6
129	A study of electronic and optical properties of NaBi(WO4)2: A disordered double tungstate crystal. Physica B: Condensed Matter, 2010, 405, 3267-3271.	2.7	10
130	Ab-initio study of electronic and optical properties of InN in wurtzite and cubic phases. Optics Communications, 2010, 283, 4655-4661.	2.1	22
131	Investigation of the Linear and Nonlinear Optical Susceptibilities of KTiOPO₄ Single Crystals: Theory and Experiment. Journal of Physical Chemistry B, 2010, 114, 16705-16712.	2.6	119
132	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.	2.6	40
133	Optical properties of bismuth germanate. Journal of Applied Physics, 2010, 107, 013514.	2.5	19
134	First-principles calculations of Born effective charges and spontaneous polarization of ferroelectric bismuth titanate. Journal of Physics Condensed Matter, 2010, 22, 165902.	1.8	27
135	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.	2.8	24
136	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.	1.5	9
137	A density functional study of second-order susceptibilities in calcium samarium oxyborate Ca₄SmO(BO₃)₃. Journal Physics D: Applied Physics, 2009, 42, 085406.	2.8	11
138	Suppression of Jahnâ€“Teller distortion by chromium and magnesium doping in spinel LiMn2O4: A first-principles study using GGA and GGA+U. Journal of Physics and Chemistry of Solids, 2009, 70, 1200-1206.	4.0	35
139	Electronic properties of orthorhombic LiGaS2 and LiGaSe2. Applied Physics A: Materials Science and Processing, 2009, 94, 315-320.	2.3	27
140	Disorder effects on electronic and optical properties of the ternary Ga_xIn_{1â^'x}P (xâ€‰=â€‰0.25, 0.50, and 0.75) alloy. Physica Status Solidi (B): Basic Research, 2009, 246, 2294-2300.	1.5	6
141	Structural, electronic and optical properties of high pressure stable phases of ZnTe. Physica B: Condensed Matter, 2009, 404, 3789-3794.	2.7	13
142	Controlled synthesis, optical and electronic properties of Eu3+ doped yttrium oxysulfide (Y2O2S) nanostructures. Journal of Colloid and Interface Science, 2009, 336, 889-897.	9.4	33
143	Electronic and magnetic behavior of ultrathin Ti nanowires. Journal of Magnetism and Magnetic Materials, 2009, 321, 1856-1862.	2.3	8
144	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.	1.8	10

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145	Band Structure, Density of States, and Optical Susceptibilities of a Novel Lithium Indium Orthoborate Li₃InB₂O₆. Journal of Physical Chemistry B, 2009, 113, 11583-11588.	2.6	8
146	Effect of U on the Electronic Properties of Neodymium Gallate (NdGaO₃): Theoretical and Experimental Studies. Journal of Physical Chemistry B, 2009, 113, 15237-15242.	2.6	53
147	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.	2.6	23
148	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.	2.5	16
149	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.	5.5	5
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