Sushil Auluck

List of Publications by Year in Descending Order

306 papers	6,021 citations	38 h-index	60 g-index
323 ext. papers	6,607 ext. citations	3.4 avg, IF	5.87 L-index

#	Paper	IF	Citations
306	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	6.1	8
305	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**,	6.7	3
304	Coupling ferroelectric polarization and anisotropic charge migration for enhanced CO2 photoreduction. *Applied Catalysis B: Environmental*, **2021**, 284, 119709	21.8	22
303	Strain induced optoelectronic properties of two dimensional MnPSe/WS heterostructure. *Journal of Physics Condensed Matter*, **2020**, 32, 315501	1.8	2
302	Optimization of electrical and thermal transport properties of Fe0.25Co0.75Sb3 Skutterudite employing the isoelectronic Bi-doping. *Intermetallics*, **2020**, 123, 106796	3.5	5
301	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	
300	Band Structure Modification and Mass Fluctuation Effects of Isoelectronic Germanium-Doping on Thermoelectric Properties of ZrNiSn. *ACS Applied Energy Materials*, **2020**, 3, 1349-1357	6.1	14
299	Enhancing gas adsorption properties of borophene by embedding transition metals. *Computational Condensed Matter*, **2020**, 22, e00436	1.7	14
298	Spin-dependent scattering induced negative magnetoresistance in topological insulator BiTe nanowires. *Scientific Reports*, **2019**, 9, 7836	4.9	8
297	Theoretical characterization of C doped SiGe monolayer. *Journal of Applied Physics*, **2019**, 125, 145703	2.5	2
296	Enhancement in thermoelectric performance of single step synthesized Mg doped Cu2Se: An experimental and theoretical study. *Intermetallics*, **2019**, 112, 106541	3.5	15
295	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	6.1	22
294	Tin doped Cu3SbSe4: A stable thermoelectric analogue for the mid-temperature applications. *Materials Research Bulletin*, **2019**, 113, 38-44	5.1	7
293	Ferroelectric polarization promoted bulk charge separation for highly efficient CO2 photoreduction of SrBi4Ti4O15. *Nano Energy*, **2019**, 56, 840-850	17.1	95
292	Magnetism by embedding 3d transition metal atoms into germanene. *Journal Physics D: Applied Physics*, **2018**, 51, 225006	3	2
291	Visible-Light-Responsive Sillén-Structured Mixed-Cationic CdBiO2Br Nanosheets: Layer Structure Design Promoting Charge Separation and Oxygen Activation Reactions. *Journal of Physical Chemistry C*, **2018**, 122, 2661-2672	3.8	51
290	Cation modified A2(Ba, Sr and Ca) ZnWO6 cubic double perovskites: A theoretical study. *Computational Condensed Matter*, **2018**, 14, 27-35	1.7	11

289	Synthesis, Crystal Structure, and Optical Gap of Two-Dimensional Halide Solid Solutions CsPb(ClBr). *Inorganic Chemistry*, **2018**, 57, 9531-9537	5.1	9
288	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	6.7	19
287	Mono and bi-layer germanene as prospective anode material for Li-ion batteries: A first-principles study. *Computational Condensed Matter*, **2018**, 16, e00314	1.7	16
286	Unexplored photoluminescence from bulk and mechanically exfoliated few layers of BiTe. *Scientific Reports*, **2018**, 8, 9205	4.9	8
285	Electronic structure, defect properties, and hydrogen storage capacity of 2H-WS2: A first-principles study. *International Journal of Hydrogen Energy*, **2018**, 43, 23126-23134	6.7	6
284	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	3.7	24
283	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	7.3	9
282	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	3.8	7
281	Role of spin-orbit interaction on the nonlinear optical response of CsPbCOF using DFT. *Physical Chemistry Chemical Physics*, **2017**, 19, 31255-31266	3.6	16
280	Thermal conductivity of thermoelectric material □Cu2Se: Implications on phonon thermal transport. *Applied Physics Letters*, **2017**, 111, 163903	3.4	9
279	An interaction potential to study the thermal structure evolution of a thermoelectric material: □Cu Se. *Journal of Computational Chemistry*, **2017**, 38, 2161-2170	3.5	12
278	Band Gap Tuning Of ZnO 1-3x N 2x F x Alloys: A First Principles Study. *Materials Today: Proceedings*, **2017**, 4, 5700-5705	1.4	1
277	Two haloid borate crystals with large nonlinear optical response. *Physical Chemistry Chemical Physics*, **2017**, 19, 18416-18425	3.6	13
276	Experimental and theoretical study of the electronic structure and optical spectral features of PbIn6Te10. *RSC Advances*, **2016**, 6, 73107-73117	3.7	5
275	Band gap engineering of ZnO substituted with nitrogen and fluorine, ZnO1□xN2xFx: a hybrid density functional study. *RSC Advances*, **2016**, 6, 99088-99095	3.7	4
274	Mg9Si5: a potential non-toxic thermoelectric material for mid-temperature applications. *RSC Advances*, **2016**, 6, 62445-62450	3.7	4
273	Luminescence and advanced mass spectroscopic characterization of sodium zinc orthophosphate phosphor for low-cost light-emitting diodes. *Luminescence*, **2016**, 31, 348-355	2.5	4
272	LiMoO3(IO3), a novel molybdenyl iodate with strong second-order optical nonlinearity. *Journal of Alloys and Compounds*, **2016**, 660, 32-38	5.7	5

271	Electrical transport and mechanical properties of thermoelectric tin selenide. *RSC Advances*, **2016**, 6, 11562-11569	3.7	40
270	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	5.7	12
269	Influence of an oxygen vacancy on the electronic structure of the asymmetric mixed borate□arbonate Pb7O(OH)3(CO3)3(BO3). *RSC Advances*, **2016**, 6, 18965-18972	3.7	1
268	Theoretical insights into kesterite and stannite phases of Cu2(Sn1□XGeX)ZnSe4 based alloys: A prospective photovoltaic material. *AIP Advances*, **2016**, 6, 125303	1.5	4
267	Stability, electronic, and optical properties of wurtzite Cu2CdxZn1□SnS4 alloys as photovoltaic materials: First-principles insight. *Physical Review B*, **2016**, 94,	3.3	9
266	Band gap engineering of CuAl1□InxS2alloys for photovoltaic applications: a first principles study. *Journal Physics D: Applied Physics*, **2016**, 49, 205103	3	4
265	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	3.7	11
264	Experimental and theoretical investigation of the electronic structure and optical properties of TlHgCl3 single crystal. *Optical Materials*, **2015**, 47, 445-452	3.3	6
263	Thermodynamical and electronic properties ofBxAl1□Nalloys: A first principle study. *Journal of Physics and Chemistry of Solids*, **2015**, 86, 101-107	3.9	13
262	Electronic structure of alkali-metal/alkaline-earth-metal fluorine beryllium borate NaSr3Be3B3O9F4 single crystal: DFT approach. *Optical Materials*, **2015**, 48, 25-30	3.3	1
261	Anisotropy and high thermopower of LaOBiS2. *Journal of Alloys and Compounds*, **2015**, 626, 208-211	5.7	9
260	Non-centrosymmetric LiBaB9O15 single crystal: growth and characterization. *Indian Journal of Physics*, **2015**, 89, 923-929	1.4	2
259	Engineering oxygen vacancies towards self-activated BaLuAl(x)Zn(4-x)O(7-(1-x)/2) photoluminescent materials: an experimental and theoretical analysis. *Physical Chemistry Chemical Physics*, **2015**, 17, 31188-94	3.6	36
258	Alkali-metal/alkaline-earth-metal fluorine beryllium borate NaSr3Be3B3O9F4 with large nonlinear optical properties in the deep-ultraviolet region. *Journal of Applied Physics*, **2015**, 117, 085703	2.5	30
257	Band gap engineering of Si-Ge alloys for mid-temperature thermoelectric applications. *AIP Advances*, **2015**, 5, 037145	1.5	9
256	An ab-initio study of CuInSe2 based ordered defect compounds. *Materials Chemistry and Physics*, **2015**, 162, 372-379	4.4	
255	Thermoelectric properties of Nowotny□uza NaZnX (X = P, As and Sb) compounds. *Computational Materials Science*, **2015**, 96, 90-95	3.2	33
254	Effects of inter-site chemical disorder on the magnetic properties of MnBi. *Journal of Magnetism and Magnetic Materials*, **2014**, 363, 18-20	2.8	9

253	Electronic band structure and specific features of AA- and AB-stacking of carbon nitride (C3N4): DFT calculation. *RSC Advances*, **2014**, 4, 6957	3.7	30
252	Thermoelectric properties of a single graphene sheet and its derivatives. *Journal of Materials Chemistry C*, **2014**, 2, 2346	7.1	58
251	A density functional study of the electronic properties of bismuth subcarbonate Bi2O2CO3. *Solid State Sciences*, **2014**, 38, 138-142	3.4	3
250	Linear and nonlinear optical properties for AA and AB stacking of carbon nitride polymorph (C3N4). *RSC Advances*, **2014**, 4, 11967-11974	3.7	27
249	Thermoelectric properties of Cu3SbSe3 with intrinsically ultralow lattice thermal conductivity. *Journal of Materials Chemistry A*, **2014**, 2, 15829-15835	13	39
248	Electronic and optical properties of chair-like and boat-like graphane. *RSC Advances*, **2014**, 4, 37411-37418	3.7	23
247	Study of ferromagnetic instability in -MnAl, using first-principles. *Journal of Alloys and Compounds*, **2014**, 601, 234-237	5.7	16
246	Linear and nonlinear optical susceptibilities of bilayer graphene. *Materials Express*, **2014**, 4, 508-520	1.3	11
245	Band structure and transport studies of copper selenide: An efficient thermoelectric material. *Applied Physics Letters*, **2014**, 105, 173905	3.4	28
244	Optical anisotropy in bismuth titanate: An experimental and theoretical study. *Journal of Applied Physics*, **2014**, 115, 133509	2.5	3
243	Adsorbing H2S onto a single graphene sheet: A possible gas sensor. *Journal of Applied Physics*, **2014** , 116, 103702	2.5	29
242	Dispersion of the linear and nonlinear optical susceptibilities of Bismuth subcarbonate Bi2O2CO3: DFT calculations. *Optical Materials*, **2014**, 38, 80-86	3.3	11
241	Dispersion of the linear and nonlinear optical susceptibilities of the CuAl(S1−xSex)2 mixed chaclcopyrite compounds. *Journal of Applied Physics*, **2014**, 116, 103501	2.5	7
240	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	2.8	8
239	An insight into evolution of electronic, magnetic, optical, and vibrational properties of ultrathin Pd nanowires. *Journal of Nanoparticle Research*, **2013**, 15, 1	2.3	4
238	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	3.2	0
237	Electronic and optical features of the mixed crystals Ag0.5Pb1.75Ge(S1−xSex)4. *Journal of Materials Chemistry C*, **2013**, 1, 4667	7.1	9
236	Room temperature nanoscale ferroelectricity in magnetoelectric GaFeO3 epitaxial thin films. *Physical Review Letters*, **2013**, 111, 087601	7.4	91

235	Optical spectra and band structure of Ag(x)Ga(x)Ge(1-x)Se2 (x = 0.333, 0.250, 0.200, 0.167) single crystals: experiment and theory. *Journal of Physical Chemistry B*, **2013**, 117, 15220-31	3.4	33
234	Linear, non-linear optical susceptibilities and the hyperpolarizability of the mixed crystals Ag(0.5)Pb(1.75)Ge(S(1-x)Se(x))4: experiment and theory. *Physical Chemistry Chemical Physics*, **2013**, 15, 18979-86	3.6	144
233	Crystallochemical affinity and optical functions of ZrGa2 and ZrGa3 compounds. *Journal of Alloys and Compounds*, **2013**, 546, 14-19	5.7	9
232	Magnetic CrX and MnX (X=Si, Ge, and As) nanowires: Stability enhancement and linearization. *Journal of Alloys and Compounds*, **2013**, 547, 138-146	5.7	1
231	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	4.3	20
230	Dispersion of the linear and nonlinear optical susceptibilities of disilver germanium sulfide from DFT calculations. *Journal of Materials Science*, **2013**, 48, 1955-1965	4.3	21
229	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, 2545-53	3.4	35
228	Band structure, density of states, and crystal chemistry of ZrGa2 and ZrGa3 single crystals. *Journal of Alloys and Compounds*, **2013**, 556, 259-265	5.7	6
227	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	4.3	6
226	Engineering polarization rotation in ferroelectric bismuth titanate. *Applied Physics Letters*, **2013**, 102, 182901	3.4	10
225	Electronic structure, charge density, and chemical bonding properties of C11H8N2O o-methoxydicyanovinylbenzene (DIVA) single crystal. *Journal of Materials Science*, **2013**, 48, 5157-5162	4.3	14
224	Mg3Sb2-based Zintl compound: a non-toxic, inexpensive and abundant thermoelectric material for power generation. *RSC Advances*, **2013**, 3, 8504	3.7	99
223	Linear and nonlinear optical susceptibilities and the hyperpolarizability of borate LiBaB9O15 single-crystal: theory and experiment. *Journal of Physical Chemistry B*, **2013**, 117, 14141-50	3.4	36
222	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	2.3	40
221	Absorption and photoconductivity spectra of AgGeS crystal: experiment and theory. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2012**, 93, 274-9	4.4	20
220	Bismuth in gallium arsenide: Structural and electronic properties of GaAs1Bix alloys. *Journal of Solid State Chemistry*, **2012**, 186, 47-53	3.3	23
219	Linear and nonlinear optical susceptibilities and hyperpolarizability of borate LiNaB4O7 single crystals: Theory and experiment. *Journal of Applied Physics*, **2012**, 112, 053526	2.5	16
218	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	2.1	9

217	Dispersion of linear, nonlinear optical susceptibilities and hyperpolarizability of C11H8N2O (o-methoxydicyanovinylbenzene) crystals. *Journal of Physical Chemistry B*, **2012**, 116, 13338-43	3.4	30
216	Implications of nanostructuring on the thermoelectric properties in half-Heusler alloys. *Applied Physics Letters*, **2012**, 101, 133103	3.4	34
215	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, 582-8	4.4	6
214	Ab initio study of magnetism in FeSe and FeTe **2012**,		3
213	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	5.7	4
212	Effect of pressure on itinerant magnetism and spin disorder in cubic FeGe. *Journal of Physics Condensed Matter*, **2012**, 24, 096003	1.8	5
211	Structural, electronic properties and charge density distribution of the LiNaB4O7: Theory and experiment. *Materials Chemistry and Physics*, **2012**, 137, 346-352	4.4	13
210	Single-crystal oxoborate (Pb3O)2(BO3)2WO4: Growth and characterization. *Materials Research Bulletin*, **2012**, 47, 2552-2560	5.1	7
209	Acentric nonlinear optical 2,4-dihydroxyl hydrazone isomorphic crystals with large linear, nonlinear optical susceptibilities and hyperpolarizability. *Journal of Physical Chemistry B*, **2012**, 116, 4677-83	3.4	40
208	Doping and temperature dependence of thermoelectric properties in Mg2(Si,Sn). *Physical Review B*, **2012**, 86,	3.3	111
207	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	10
206	Chalcogen height dependence of magnetism and Fermiology in FeTexSe1□. *Superconductor Science and Technology*, **2012**, 25, 095002	3.1	17
205	Linear optical susceptibilities of the oxoborate (Pb3O)2(BO3)2WO4: theory and experiment. *Journal of Materials Science*, **2012**, 47, 5794-5800	4.3	3
204	Photoconducting state and its perturbation by electrostatic fields in oxide-based two-dimensional electron gas. *Physical Review B*, **2012**, 86,	3.3	43
203	Electronic and vibrational properties of vanadium-carbide nanowires. *Journal of Applied Physics*, **2012**, 112, 063502	2.5	2
202	Electronic and optical properties of free-standing and supported vanadium nanowires. *Journal of Applied Physics*, **2012**, 111, 093506	2.5	8
201	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	22
200	Effect of site-disorder on magnetism and magneto-structural coupling in gallium ferrite: A first-principles study. *Journal of Applied Physics*, **2012**, 111, 043915	2.5	12

199	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, 2836-41	3.4	34
198	Normal state and superconducting properties of Rh17S15and Pd17Se15. *Superconductor Science and Technology*, **2011**, 24, 105015	3.1	8
197	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, 2945-52	3.6	148
196	Electronic structure, chemical bonding features, and electron charge density of the double-cubane single crystal [Sb7S8Br2](AlCl4)3. *Applied Physics Letters*, **2011**, 98, 201903	3.4	14
195	Density functional calculations, electronic structure, and optical properties of molybdenum bimetallic nitrides Pt2Mo3N and Pd2Mo3N. *Journal of Physical Chemistry B*, **2011**, 115, 3363-70	3.4	6
194	Effect of increasing tellurium content on the electronic and optical properties of cadmium selenide telluride alloys CdSe1−xTex: An ab initio study. *Journal of Alloys and Compounds*, **2011**, 509, 6737-6750	5.7	39
193	Bismuth-containing semiconductors: Linear and nonlinear optical susceptibilities of GaAs1−xBix alloys. *Journal of Alloys and Compounds*, **2011**, 509, 9685-9691	5.7	31
192	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		42
191	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	3.9	10
190	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	4.4	9
189	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	4.4	16
188	Energetics and electronic structure of La/Sr disorder at the interface of SrTiO3/LaTiO3 heterostructure. *Applied Physics Letters*, **2011**, 99, 081915	3.4	4
187	Second harmonic generation and hyperpolarizabilities of the double-cubane compound [Sb7S8Br2](AlCl4)3: chalcogenide in ionic liquids. *Journal of Physical Chemistry B*, **2011**, 115, 11763-9	3.4	13
186	First-principles comparison of the cubic and tetragonal phases of. *Chemical Physics Letters*, **2011**, 504, 148-152	2.5	3
185	Structural, thermodynamic and optical properties of MgF2 studied from first-principles theory. *Journal of Solid State Chemistry*, **2011**, 184, 343-350	3.3	60
184	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	3.3	4
183	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	10
182	Electronic structure, Born effective charges and spontaneous polarization in magnetoelectric gallium ferrite. *Journal of Physics Condensed Matter*, **2011**, 23, 325902	1.8	31

181	Physical property and electronic structure characterization of bulk superconducting Bi3Ni. *Superconductor Science and Technology*, **2011**, 24, 085002	3.1	29
180	Investigation of the linear and nonlinear optical susceptibilities of KTiOPO4 single crystals: theory and experiment. *Journal of Physical Chemistry B*, **2010**, 114, 16705-12	3.4	97
179	Linear and nonlinear optical susceptibilities of 3-phenylamino-4-phenyl-1,2,4-triazole-5-thione. *Journal of Physical Chemistry B*, **2010**, 114, 1815-21	3.4	36
178	Optical properties of bismuth germanate. *Journal of Applied Physics*, **2010**, 107, 013514	2.5	16
177	First-principles calculations of Born effective charges and spontaneous polarization of ferroelectric bismuth titanate. *Journal of Physics Condensed Matter*, **2010**, 22, 165902	1.8	21
176	Density functional calculations of the electronic structure of 3-phenylamino-4-phenyl-1,2,4-triazole-5-thione. *Physical Chemistry Chemical Physics*, **2010**, 12, 2975-80	3.6	22
175	Theoretical studies on electronic and magnetic properties of ultrathin Mo nanowires. *Journal of Applied Physics*, **2010**, 107, 024307	2.5	3
174	Optical and magneto-optical properties of Fe4□Cox (x = 1□). *European Physical Journal B*, **2010**, 73, 423-432	1.2	6
173	A study of electronic and optical properties of NaBi(WO4)2: A disordered double tungstate crystal. *Physica B: Condensed Matter*, **2010**, 405, 3267-3271	2.8	5
172	Ab-initio study of electronic and optical properties of InN in wurtzite and cubic phases. *Optics Communications*, **2010**, 283, 4655-4661	2	16
171	Comparison of the Density of States Obtained from the X-ray Photoelectron Spectra with the Electronic Structure Calculations for □BiB3O6. *Japanese Journal of Applied Physics*, **2009**, 48, 011601	1.4	9
170	A density functional study of second-order susceptibilities in calcium samarium oxyborate Ca4SmO(BO3)3. *Journal Physics D: Applied Physics*, **2009**, 42, 085406	3	9
169	Suppression of Jahn□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	3.9	30
168	Electronic properties of orthorhombic LiGaS2 and LiGaSe2. *Applied Physics A: Materials Science and Processing*, **2009**, 94, 315-320	2.6	22
167	Disorder effects on electronic and optical properties of the ternary GaxIn1□P (x = 0.25, 0.50, and 0.75) alloy. *Physica Status Solidi (B): Basic Research*, **2009**, 246, 2294-2300	1.3	4
166	Structural, electronic and optical properties of high pressure stable phases of ZnTe. *Physica B: Condensed Matter*, **2009**, 404, 3789-3794	2.8	10
165	Controlled synthesis, optical and electronic properties of Eu3+ doped yttrium oxysulfide (Y2O2S) nanostructures. *Journal of Colloid and Interface Science*, **2009**, 336, 889-97	9.3	28
164	Electronic and magnetic behavior of ultrathin Ti nanowires. *Journal of Magnetism and Magnetic Materials*, **2009**, 321, 1856-1862	2.8	8

163	Synthesis, IR, UV-vis spectra, x-ray diffraction and band structure of a non-centrosymmetric borate single-crystal CaBiGaB(2)O(7). *Journal of Physics Condensed Matter*, **2009**, 21, 205402	1.8	9
162	Band structure, density of states, and optical susceptibilities of a novel lithium indium orthoborate Li3InB2O6. *Journal of Physical Chemistry B*, **2009**, 113, 11583-8	3.4	8
161	Effect of U on the electronic properties of neodymium gallate (NdGaO3): theoretical and experimental studies. *Journal of Physical Chemistry B*, **2009**, 113, 15237-42	3.4	43
160	X-ray photoelectron spectrum and electronic properties of a noncentrosymmetric chalcopyrite compound HgGa(2)S(4): LDA, GGA, and EV-GGA. *Journal of Physical Chemistry B*, **2009**, 113, 5803-8	3.4	21
159	Dispersion of linear and nonlinear optical susceptibilities in calcium neodymium oxyborate Ca4NdO(BO3)3-LDA versus GGA. *Journal of Physical Chemistry A*, **2009**, 113, 1614-22	2.8	14
158	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	5.7	5
157	Several features of nonlinear optical susceptibilities of LiGaX2 (X = S, Se) ternary compounds. *Journal of Alloys and Compounds*, **2009**, 473, 20-24	5.7	36
156	Optical properties and critical points in ordered BexZn1−xSe alloys. *Journal of Alloys and Compounds*, **2009**, 480, 717-722	5.7	7
155	Magneto-optical properties of transition metal compounds XPt3 (X=V, Cr, Mn, Fe, Co) and X3Pt (X=Fe, Co). *Journal of Alloys and Compounds*, **2009**, 486, 60-65	5.7	10
154	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, 6640-6	3.4	7
153	Ab initio calculation of the electronic band structure, density of states and optical properties of alpha-2-methyl-1-nitroisothiourea. *Journal of Physical Chemistry B*, **2009**, 113, 12648-54	3.4	14
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