Ali Hussain Reshak

List of Publications by Citations

454 papers	9,926 citations	45 h-index	75 g-index
473 ext. papers	11,143 ext. citations	3.8 avg, IF	6.99 L-index

#	Paper	IF	Citations
454	Macroscopic Polarization Enhancement Promoting Photo- and Piezoelectric-Induced Charge Separation and Molecular Oxygen Activation. *Angewandte Chemie - International Edition*, **2017**, 56, 11860-11864	16.4	662
453	Chlorine intercalation in graphitic carbon nitride for efficient photocatalysis. *Applied Catalysis B: Environmental*, **2017**, 203, 465-474	21.8	241
452	Elastic, electronic and optical properties of ZnS, ZnSe and ZnTe under pressure. *Computational Materials Science*, **2006**, 38, 29-38	3.2	230
451	Photoelectrical properties and the electronic structure of Tl(1-x)In(1-x)Sn(x)Se2 (x = 0, 0.1, 0.2, 0.25) single crystalline alloys. *Physical Chemistry Chemical Physics*, **2013**, 15, 6965-72	3.6	156
450	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
449	Ab initio study of TaON, an active photocatalyst under visible light irradiation. *Physical Chemistry Chemical Physics*, **2014**, 16, 10558-65	3.6	145
448	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
447	Fe2MnSixGe1□: influence thermoelectric properties of varying the germanium content. *RSC Advances*, **2014**, 4, 39565-39571	3.7	143
446	Thermoelectric properties for AA- and AB-stacking of a carbon nitride polymorph (C3N4). *RSC Advances*, **2014**, 4, 63137-63142	3.7	138
445	FP-APW+lo calculations of the elastic properties in zinc-blende III-P compounds under pressure effects. *Computational Materials Science*, **2009**, 45, 474-479	3.2	123
444	Spin-polarized Second Harmonic Generation from the Antiferromagnetic CaCoSO Single Crystal. *Scientific Reports*, **2017**, 7, 46415	4.9	116
443	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
442	Ab initio study of structural, electronic, elastic and high pressure properties of barium chalcogenides. *Computational Materials Science*, **2006**, 38, 263-270	3.2	97
441	Ferroelectric polarization promoted bulk charge separation for highly efficient CO2 photoreduction of SrBi4Ti4O15. *Nano Energy*, **2019**, 56, 840-850	17.1	95
440	Thickness dependence of structural, electrical and optical behaviour of undoped ZnO thin films. *Physica B: Condensed Matter*, **2008**, 403, 3326-3330	2.8	94
439	Ab-initio calculations of Co-based diluted magnetic semiconductors Cd1□CoxX (X=S, Se, Te). *Journal of Magnetism and Magnetic Materials*, **2010**, 322, 3214-3222	2.8	92
438	Second order optical effects in Au´nanoparticle-deposited ZnO nanocrystallite films. *Nanotechnology*, **2008**, 19, 185709	3.4	87

437	Band energy and thermoelectricity of filled skutterudites LaFe4Sb12 and CeFe4Sb12. *Journal of Alloys and Compounds*, **2007**, 437, 39-46	5.7	80
436	Theoretical study of mechanical, electronic, chemical bonding and optical properties of Ti2SnC, Zr2SnC, Hf2SnC and Nb2SnC. *Computational Materials Science*, **2009**, 47, 491-500	3.2	77
435	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	1.3	77
434	Calculated optical properties of 2H MoS2 intercalated with lithium. *Physical Review B*, **2003**, 68,	3.3	75
433	Electronic and optical properties of the 1T phases of TiS2, TiSe2, and TiTe2. *Physical Review B*, **2003**, 68,	3.3	73
432	Variation of half metallicity and magnetism of Cd1 CrxZ (Z=S, Se and Te) DMS compounds on reducing dilute limit. *Journal of Magnetism and Magnetic Materials*, **2013**, 331, 1-6	2.8	71
431	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	5.7	67
430	Electronic structure, magnetism and robust half-metallicity of new quaternary Heusler alloy FeCrMnSb. *Journal of Alloys and Compounds*, **2013**, 580, 201-204	5.7	62
429	First-principles calculations of the elastic, electronic, and optical properties of the filled skutterudites CeFe4P12 and ThFe4P12. *Physical Review B*, **2007**, 75,	3.3	62
428	Structural and optical insights to enhance solar cell performance of CdS nanostructures. *Energy Conversion and Management*, **2014**, 82, 238-243	10.6	60
427	First-principles calculations of structural, elastic and electronic properties of Ni2MnZ (Z = Al, Ga and In) Heusler alloys. *Physica Status Solidi (B): Basic Research*, **2009**, 246, 1580-1586	1.3	59
426	Thermoelectric properties of a single graphene sheet and its derivatives. *Journal of Materials Chemistry C*, **2014**, 2, 2346	7.1	58
425	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	2.3	58
424	An ab initio study of the electronic structure and optical properties of CdS1 e alloys. *Solar Energy*, **2010**, 84, 1979-1984	6.8	57
423	Role of titanium valence states in optical and electronic features of PbO Sb2O3 B2O3:TiO2 glass alloys. *Journal of Alloys and Compounds*, **2009**, 482, 283-297	5.7	55
422	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	12	54
421	Theoretical investigation of the electronic properties, and first and second harmonic generation for cadmium chalcogenide. *Journal of Chemical Physics*, **2006**, 124, 104707	3.9	53
420	Exploration of the Electronic Structure of Monoclinic Eu2(MoO4)3: DFT-Based Study and X-ray Photoelectron Spectroscopy. *Journal of Physical Chemistry C*, **2016**, 120, 10559-10568	3.8	52

419	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
418	Linear, nonlinear optical properties and birefringence of AgGaX2 (X=S, Se, Te) compounds. *Physica B: Condensed Matter*, **2005**, 369, 243-253	2.8	50
417	Emergence of half metallicity in Cr-doped GaP dilute magnetic semiconductor compound within solubility limit. *Journal of Alloys and Compounds*, **2012**, 536, 214-218	5.7	49
416	First-principle calculations of the linear and nonlinear optical response for GaX (X = As, Sb, P). *European Physical Journal B*, **2005**, 47, 503-508	1.2	49
415	Specific features in the band structure and linear and nonlinear optical susceptibilities of La2CaB10O19 crystals. *Physical Review B*, **2007**, 75,	3.3	48
414	Electronic spectral parameters and IR nonlinear optical features of novel Ag0.5Pb1.75GeS4 crystal. *Journal of Crystal Growth*, **2012**, 354, 142-146	1.6	46
413	First-principles study of spin-polarized electronic band structures in ferromagnetic Zn1−xTMxS (TM=Fe, Co and Ni). *Journal of Alloys and Compounds*, **2010**, 508, 245-250	5.7	46
412	Linear and nonlinear optical susceptibilities for a novel borate oxide BaBiBO4: Theory and experiment. *Journal of Solid State Chemistry*, **2008**, 181, 789-795	3.3	46
411	Electronic, linear, and nonlinear optical properties of III-V indium compound semiconductors. *Journal of Chemical Physics*, **2006**, 125, 34710	3.9	46
410	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	3.7	45
409	Elastic properties and bonding of the AgGaSe2 chalcopyrite. *Physica B: Condensed Matter*, **2010**, 405, 3658-3664	2.8	45
408	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
407	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	12	43
406	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	2.8	43
405	Structural, mechanical and electronic properties of sodium based fluoroperovskites NaXF3 (X=Mg, Zn) from first-principle calculations. *Materials Science in Semiconductor Processing*, **2015**, 33, 127-135	4.3	42
404	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
403	Band structure and optical response of 2H-MoX2 compounds (X=S, Se, and Te). *Physical Review B*, **2005**, 71,	3.3	42
402	Elastic, electronic and optical properties of cubic antiperovskites SbNCa3 and BiNCa3. *Computational Materials Science*, **2009**, 46, 1051-1057	3.2	41

401	Ab initio calculations of the electronic, linear and nonlinear optical properties of zinc chalcogenides. *Physica B: Condensed Matter*, **2007**, 388, 34-42	2.8	41
400	Specific features of electronic structures and optical susceptibilities of molybdenum oxide. *RSC Advances*, **2015**, 5, 22044-22052	3.7	40
399	Ab initio method of optical investigations of CdS 1□x Te x alloys under quantum dots diameter effect. *Solar Energy*, **2015**, 115, 33-39	6.8	40
398	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
397	Accounting oxygen vacancy for half-metallicity and magnetism in Fe-doped CeO2 dilute magnetic oxide. *Computational Materials Science*, **2013**, 74, 114-118	3.2	40
396	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
395	Effect of increasing tellurium content on the electronic and optical properties of cadmium selenide telluride alloys CdSe1□Tex: An ab initio study. *Journal of Alloys and Compounds*, **2011**, 509, 6737-6750	5.7	39
394	Theoretical investigation of the electronic and optical properties of ZrX2 (X=S, Se and Te). *Physica B: Condensed Matter*, **2004**, 353, 230-237	2.8	39
393	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	1.6	38
392	Spin-polarized structural, electronic, and magnetic properties of diluted magnetic semiconductors Cd(1-x)Mn(x)S and Cd(1-x)Mn(x)Se in zinc blende phase. *Journal of Physical Chemistry A*, **2009**, 113, 6022-7	2.8	38
391	Theoretical investigations of NiTiSn and CoVSn compounds. *Journal of Physics and Chemistry of Solids*, **2012**, 73, 975-981	3.9	37
390	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
389	Structural, chemical bonding, electronic and magnetic properties of KMF3 (M=Mn, Fe, Co, Ni) compounds. *Computational Materials Science*, **2014**, 85, 402-408	3.2	36
388	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
387	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
386	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
385	Density functional study of optical properties of beryllium chalcogenides compounds in nickel arsenide B8 structure. *Physica B: Condensed Matter*, **2012**, 407, 286-296	2.8	35
384	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

383	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
382	Thermoelectric properties of Nowotny□uza NaZnX (X = P, As and Sb) compounds. *Computational Materials Science*, **2015**, 96, 90-95	3.2	33
381	Active photocatalytic water splitting solar-to-hydrogen energy conversion: Chalcogenide photocatalyst Ba2ZnSe3 under visible irradiation. *Applied Catalysis B: Environmental*, **2018**, 221, 17-26	21.8	33
380	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
379	GGA+U studies of the cubic perovskites BaMO3 (M=Pr, Th and U). *Physica B: Condensed Matter*, **2013**, 410, 217-221	2.8	33
378	Electronic structure and optical properties of 1T-TiS2 and lithium intercalated 1T-TiS2 for lithium batteries. *Journal of Chemical Physics*, **2008**, 129, 074706	3.9	33
377	First and second harmonic generation of the optical susceptibilities for the non-centro-symmetric orthorhombic AgCd2GaS4. *Journal of Physics Condensed Matter*, **2008**, 20, 325234	1.8	33
376	Third harmonic generation process in Al doped ZnO thin films. *Journal of Alloys and Compounds*, **2014**, 584, 7-12	5.7	32
375	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	5.7	32
374	Photoinduced effects in l-alanine crystals. *Materials Letters*, **2010**, 64, 1957-1959	3.3	32
373	Evidence of Coulomb correction and spin□rbit coupling in rare-earth dioxides CeO2, PrO2 and TbO2: An ab initio study. *Journal of Magnetism and Magnetic Materials*, **2012**, 324, 1397-1405	2.8	31
372	Bismuth-containing semiconductors: Linear and nonlinear optical susceptibilities of GaAs1□Bix alloys. *Journal of Alloys and Compounds*, **2011**, 509, 9685-9691	5.7	31
371	Photoinduced effects in TiO2 nanocrystalline films with different morphology. *Journal of Alloys and Compounds*, **2010**, 508, 599-605	5.7	31
370	Ab-initio study of the structural, linear and nonlinear optical properties of CdAl2Se4 defect-chalcopyrite. *Journal of Solid State Chemistry*, **2010**, 183, 46-51	3.3	31
369	Investigation of the electronic properties, first and second harmonic generation for AXIIIBXV zinc-blende semiconductors. *Physica B: Condensed Matter*, **2007**, 395, 143-150	2.8	31
368	Electronic properties of chalcopyrite CuAlX2(X=S,Se,Te) compounds. *Solid State Communications*, **2008**, 145, 571-576	1.6	31
367	Synthesis, Structural, Thermal, and Electronic Properties of Palmierite-Related Double Molybdate □CsPb(MoO). *Inorganic Chemistry*, **2017**, 56, 3276-3286	5.1	30
366	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

365	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
364	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
363	Electro-structural correlations, elastic and optical properties among the nanolaminated ternary carbides Zr2AC. *Solid State Sciences*, **2010**, 12, 887-898	3.4	30
362	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	2.6	30
361	Structural, electronic and optical properties of fluorite-type compounds. *European Physical Journal B*, **2005**, 47, 63-70	1.2	30
360	Adsorbing H2S onto a single graphene sheet: A possible gas sensor. *Journal of Applied Physics*, **2014** , 116, 103702	2.5	29
359	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	3.3	29
358	Structural and electronic properties of GaN x As1 alloys. *Applied Physics A: Materials Science and Processing*, **2012**, 106, 687-696	2.6	28
357	X-ray diffraction and optical properties of a noncentrosymmetric borate CaBiGaB(2)O(7). *Journal of Chemical Physics*, **2008**, 129, 204111	3.9	28
356	Linear and nonlinear optical properties for AA and AB stacking of carbon nitride polymorph (C3N4). *RSC Advances*, **2014**, 4, 11967-11974	3.7	27
355	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	3.6	27
354	Ab-initio calculation of structural, electronic, and optical characterizations of the intermetallic trialuminides ScAl3 compound. *Journal of Solid State Chemistry*, **2010**, 183, 1290-1296	3.3	27
353	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	5.7	26
352	Effect of cation substitution on electronic band structure of ZnGeAs2 pnictides: A mBJLDA approach. *Journal of Alloys and Compounds*, **2012**, 518, 74-79	5.7	26
351	Prediction study of the structural, elastic and high pressure properties of Yttrium chalcogenide. *Computational Materials Science*, **2010**, 49, 372-377	3.2	26
350	Prediction study of the structural and elastic properties for the cubic skutterudites LaFe4A12 (A´= ´P, As and Sb) under pressure effect. *Solid State Communications*, **2010**, 150, 1869-1873	1.6	26
349	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	1.2	26
348	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	6.7	25

347	Phase transition of LaX (X = P, As, Sb and Bi) at high pressure: Theoretical investigation of the structural and electronic properties. *Solid State Communications*, **2008**, 148, 139-144	1.6	25
346	Electronic band structure of AgCd2GaS4: theory and experiment. *Journal of Physics Condensed Matter*, **2008**, 20, 325213	1.8	25
345	Ab initio calculations of the electronic and optical properties of 1T-HfX2 compounds. *Physica B: Condensed Matter*, **2005**, 363, 25-31	2.8	25
344	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	1.5	25
343	Two symmetric n-type interfaces SrTiO3/LaAlO3 in perovskite: Electronic properties from density functional theory. *Journal of Applied Physics*, **2016**, 119, 245303	2.5	25
342	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
341	Transport properties of g-BC3 and t-BC3 phases. *RSC Advances*, **2015**, 5, 33632-33638	3.7	24
340	Quest for magnetism in graphene via Cr- and Mo-doping: A DFT approach. *Physica E: Low-Dimensional Systems and Nanostructures*, **2016**, 78, 35-40	3	24
339	Structural, Elastic, Electronic and Optical Properties of Cu3TMSe4 (TM = V, Nb and Ta) Sulvanite Compounds via First-Principles Calculations. *Science of Advanced Materials*, **2013**, 5, 97-106	2.3	24
338	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	5.7	23
337	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	4.3	23
336	Electronic and optical properties of chair-like and boat-like graphane. *RSC Advances*, **2014**, 4, 37411-37418	3.7	23
335	Optical and photoconductivity spectra of novel AgInSiS$_2$ and AgInGeS$_2$ chalcogenide crystals. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2012**, 91, 48-50	4.4	23
334	Bismuth in gallium arsenide: Structural and electronic properties of GaAs1−xBix alloys. *Journal of Solid State Chemistry*, **2012**, 186, 47-53	3.3	23
333	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	2.8	23
332	FP-LAPW investigation of structural, electronic, linear and nonlinear optical properties of ZnIn2Te4 defect-chalcopyrite. *Computational Materials Science*, **2010**, 50, 651-655	3.2	23
331	FP-APW+lo calculations of the electronic and optical properties of alkali metal sulfides under pressure. *Journal of Physics Condensed Matter*, **2009**, 21, 095404	1.8	23
330	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	2.8	23

329	Theoretical investigation of the structural, electronic, magnetic and elastic properties of binary cubic C15-Laves phases TbX2 (X = Co and Fe). *Journal of Alloys and Compounds*, **2016**, 689, 885-893	5.7	23
328	Electronic, optical, and thermoelectric properties of Fe2+xV1−xAl. *AIP Advances*, **2017**, 7, 045118	1.5	22
327	Electronic and optical properties of pentagonal-B2C monolayer: A first-principles calculation. *International Journal of Modern Physics B*, **2017**, 31, 1750044	1.1	22
326	Density of electronic states and dispersion of optical functions of defect chalcopyrite CdGa2X4 (X = S, Se): DFT study. *Materials Research Bulletin*, **2013**, 48, 4555-4564	5.1	22
325	Analytical investigations of CdS nanostructures for optoelectronic applications. *Optik*, **2015**, 126, 5109-5114	1.5	22
324	Electronic band structure and specific features of Sm2NiMnO6 compound: DFT calculation. *Journal of Magnetism and Magnetic Materials*, **2013**, 342, 80-86	2.8	22
323	Calculated optical properties of GaX (X=P, As, Sb) under hydrostatic pressure. *Applied Physics A: Materials Science and Processing*, **2011**, 104, 1159-1167	2.6	22
322	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
321	Electronic properties of orthorhombic LiGaS2 and LiGaSe2. *Applied Physics A: Materials Science and Processing*, **2009**, 94, 315-320	2.6	22
320	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, 281-5	4.4	22
319	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	12	22
318	UV-excited piezo-optical effects in oxide nanocrystals incorporated into PMMA matrices. *Acta Materialia*, **2008**, 56, 5677-5684	8.4	22
317	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	1.6	22
316	Coupling ferroelectric polarization and anisotropic charge migration for enhanced CO2 photoreduction. *Applied Catalysis B: Environmental*, **2021**, 284, 119709	21.8	22
315	Transport properties of mixed CuAl(S1−xSex)2 as promising thermoelectric crystalline materials. *Journal of Physics and Chemistry of Solids*, **2015**, 78, 46-52	3.9	21
314	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	3.8	21
313	Investigation of electronic structure and optical properties of MgAl2O4: DFT approach. *Optical Materials*, **2014**, 37, 322-326	3.3	21
312	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

311	First-Principles Study on the Structural, Electronic, Magnetic and Thermodynamic Properties of Full Heusler Alloys Co2VZ (Z = Al, Ga). *Journal of Electronic Materials*, **2017**, 46, 130-142	1.9	21
310	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	3.2	21
309	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
308	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	5.7	21
307	First principles calculations of electronic structure and magnetic properties of Cr-based magnetic semiconductors Al1−xCrxX (X=N, P, As, Sb). *Journal of Solid State Chemistry*, **2010**, 183, 242-249	3.3	21
306	Photoinduced non-linear optical effects in lanthanum calcium borate single crystals. *Journal of Materials Science*, **2006**, 41, 1927-1932	4.3	21
305	Thermoelectric properties of highly-mismatched alloys of GaNxAs1−x from first- to second-principles methods: energy conversion. *RSC Advances*, **2016**, 6, 72286-72294	3.7	21
304	Absorption and photoconductivity spectra of AgGaSe2 crystal: experiment and theory. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2012**, 93, 274-9	4.4	20
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