Iftikhar Ahmad

List of Publications by Citations

230 papers	3,610 citations	30 h-index	48 g-index
241 ext. papers	4,591 ext. citations	2.7 avg, IF	5.89 L-index

#	Paper	IF	Citations
230	Elastic constants of cubic crystals. *Computational Materials Science*, **2014**, 95, 592-599	3.2	192
229	First principle study of the structural and optoelectronic properties of cubic perovskites CsPbM3 (M=Cl, Br, I). *Physica B: Condensed Matter*, **2011**, 406, 3222-3229	2.8	178
228	Ab initio study of the bandgap engineering of Al1−xGaxN for optoelectronic applications. *Journal of Applied Physics*, **2011**, 109, 023109	2.5	129
227	Structural, electronic and optical properties of CsPbX3 (X=Cl, Br, I) for energy storage and hybrid solar cell applications. *Journal of Alloys and Compounds*, **2017**, 705, 828-839	5.7	119
226	Rashba spin splitting and photocatalytic properties of GeCrMSSe (M=Mo, W) van der Waals heterostructures. *Physical Review B*, **2019**, 100,	3.3	92
225	Investigation of structural and optoelectronic properties of BaThO3. *Optical Materials*, **2011**, 33, 553-557	3.3	87
224	Optoelectronic and solar cell applications of Janus monolayers and their van der Waals heterostructures. *Physical Chemistry Chemical Physics*, **2019**, 21, 18612-18621	3.6	77
223	Ab initio calculations of structural, optical and thermoelectric properties for CoSb3 and ACo4Sb12 (A = La, Tl and Y) compounds. *Computational Materials Science*, **2012**, 65, 509-519	3.2	74
222	IRelast package. *Journal of Alloys and Compounds*, **2018**, 735, 569-579	5.7	62
221	Electronic structure, optical and photocatalytic performance of SiC-MX (M = Mo, W and X = S, Se) van der Waals heterostructures. *Physical Chemistry Chemical Physics*, **2018**, 20, 24168-24175	3.6	60
220	Direct ultraviolet excitation of an amorphous AlN:praseodymium phosphor by codoped Gd3+ cathodoluminescence. *Applied Physics Letters*, **2007**, 91, 193511	3.4	58
219	Thermoelectric properties of SbNCa3 and BiNCa3 for thermoelectric devices and alternative energy applications. *Computer Physics Communications*, **2014**, 185, 1394-1398	4.2	53
218	Conversion of Direct to Indirect Bandgap and Optical Response of B Substituted InN for Novel Optical Devices Applications. *Journal of Lightwave Technology*, **2010**, 28, 223-227	4	47
217	Van der Waals heterostructures of P, BSe, and SiC monolayers. *Journal of Applied Physics*, **2019**, 125, 094301	2.5	45
216	Opto-electronic response of spinels MgAl2O4 and MgGa2O4 through modified Becke-Johnson exchange potential. *Physica B: Condensed Matter*, **2012**, 407, 2588-2592	2.8	45
215	Intriguing electronic structures and optical properties of two-dimensional van der Waals heterostructures of Zr2CT2 (T = O, F) with MoSe2 and WSe2. *Journal of Materials Chemistry C*, **2018**, 6, 2830-2839	7.1	43
214	First principle studies of structural, elastic, electronic and optical properties of Zn-chalcogenides under pressure. *Journal of Semiconductors*, **2014**, 35, 072001	2.3	43

213	Electronic structure of cubic perovskite SnTaO3. *Intermetallics*, **2012**, 31, 287-291	3.5	41
212	Strain engineering of electronic structures and photocatalytic responses of MXenes functionalized by oxygen. *Physical Chemistry Chemical Physics*, **2017**, 19, 14738-14744	3.6	40
211	Cr-Doped III□V Nitrides: Potential Candidates for Spintronics. *Journal of Electronic Materials*, **2011**, 40, 1428-1436	1.9	38
210	Thermoelectric studies of IV□VI semiconductors for renewable energy resources. *Materials Science in Semiconductor Processing*, **2016**, 48, 85-94	4.3	36
209	Structural and optoelectronic properties of the zinc titanate perovskite and spinel by modified Becke□ohnson potential. *Physica B: Condensed Matter*, **2013**, 420, 54-57	2.8	36
208	Effect of phase transition on the optoelectronic properties of Zn1□MgxS. *Journal of Applied Physics*, **2012**, 112, 073104	2.5	36
207	Shift of indirect to direct bandgap and optical response of LaAlO3 under pressure. *Journal of Applied Physics*, **2012**, 111, 123116	2.5	36
206	Theoretical studies of structural and magnetic properties of cubic perovskites PrCoO3 and NdCoO3. *Physica B: Condensed Matter*, **2011**, 406, 3800-3804	2.8	36
205	On the Morphology and Composition of Particulate Matter in an Urban Environment. *Aerosol and Air Quality Research*, **2018**, 18, 1431-1447	4.6	36
204	GGA+U studies of the cubic perovskites BaMO3 (M=Pr, Th and U). *Physica B: Condensed Matter*, **2013**, 410, 217-221	2.8	33
203	Robust half-metallicity in Ga1-xMnxP and Ga1-xMnxAs. *Computational Materials Science*, **2013**, 68, 55-60	3.2	32
202	Electronic and optical properties of mixed Be-chalcogenides. *Journal of Physics and Chemistry of Solids*, **2013**, 74, 181-188	3.9	32
201	Conversion of optically isotropic to anisotropic CdSxSe1□ (0?x?1) alloy with S concentration. *Computational Materials Science*, **2013**, 77, 145-152	3.2	32
200	Morphological, Raman, electrical and dielectric properties of rare earth doped X-type hexagonal ferrites. *Physica B: Condensed Matter*, **2016**, 503, 38-43	2.8	30
199	Bandgap investigations and the effect of the In and Al concentration on the optical properties of In_xAl_1□N. *Journal of the Optical Society of America B: Optical Physics*, **2009**, 26, 2181	1.7	30
198	Theoretical investigation of half metallicity in Fe/Co/Ni doped ZnSe material systems. *Journal of Applied Physics*, **2009**, 106, 093710	2.5	30
197	Theoretical studies of the paramagnetic perovskites MTaO3 (M = Ca, Sr and Ba). *Materials Chemistry and Physics*, **2015**, 162, 308-315	4.4	29
196	Antiperovskite compounds SbNSr3 and BiNSr3: Potential candidates for thermoelectric renewable energy generators. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2015**, 379, 206-210	2.3	29

195	Gray-box modeling for prediction and control of molten steel temperature in tundish. *Journal of Process Control*, **2014**, 24, 375-382	3.9	29
194	Structural and Optoelectronic Properties of Cubic CsPbF 3 for Novel Applications. *Chinese Physics Letters*, **2011**, 28, 117803	1.8	28
193	Metal mono-chalcogenides ZnX and CdX (X = S, Se and Te) monolayers: Chemical bond and optical interband transitions by first principles calculations. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2017**, 381, 663-670	2.3	27
192	Structural, electronic and optical properties of CaxCd1−xO and its conversion from semimetal to wide bandgap semiconductor. *Computational Materials Science*, **2012**, 58, 71-76	3.2	27
191	Structural and optoelectronic properties of Mg substituted ZTe (Z=Zn, Cd and Hg). *Journal of Physics and Chemistry of Solids*, **2015**, 83, 75-84	3.9	26
190	First principle study of cubic perovskites: AgTF3 (T=Mg, Zn). *Physica B: Condensed Matter*, **2011**, 406, 4584-4589	2.8	26
189	Structural and thermoelectric properties of pure and La, Y doped HoMnO3 for their use as alternative energy materials. *Computer Physics Communications*, **2015**, 187, 1-7	4.2	25
188	Investigation of half metallicity in Fe doped CdSe and Co doped CdSe materials. *Current Applied Physics*, **2012**, 12, 184-187	2.6	25
187	Bandgap engineering of Cd1−xSrxO. *Physica B: Condensed Matter*, **2011**, 406, 2509-2514	2.8	25
186	Electronic Band Structures of the Highly Desirable III–V Semiconductors: TB-mBJ DFT Studies. *Journal of Electronic Materials*, **2016**, 45, 3314-3323	1.9	25
185	Theoretical studies of strongly correlated rare-earth intermetallics RIn3 and RSn3 (R = Sm, Eu, and Gd). *Journal of Applied Physics*, **2014**, 116, 103905	2.5	24
184	Electronic Properties of Antiperovskite Materials from State-of-the-Art Density Functional Theory. *Journal of Chemistry*, **2015**, 2015, 1-11	2.3	24
183	Transition from optically inactive to active Mg-chalcogenides: A first principle study. *Computational Materials Science*, **2012**, 61, 278-282	3.2	24
182	The investigation of spherical effects on the photodetached electron spectra. *Journal of Physics B: Atomic, Molecular and Optical Physics*, **2011**, 44, 195004	1.3	24
181	Theoretical studies of the band structure and optoelectronic properties of ZnOxS1−x. *International Journal of Quantum Chemistry*, **2013**, 113, 1285-1292	2.1	23
180	Band Profile Comparison of the Cubic Perovskites CaCoO3 and SrCoO3. *Journal of Electronic Materials*, **2013**, 42, 438-444	1.9	23
179	Electronic Structure of Crystalline Buckyballs: fcc-C60. *Journal of Electronic Materials*, **2016**, 45, 339-348	1.9	22
178	Elastic and mechanical properties of lanthanide monoxides. *Journal of Alloys and Compounds*, **2015**, 618, 292-298	5.7	22

177	Shift of indirect to direct bandgap in going from K to Cs in MCaF3 (M□=□K, Rb, Cs). *Solid State Sciences*, **2013**, 16, 152-157	3.4	21
176	Thermoelectric and phononic properties of (Gd, Tb) MnO3 compounds: DFT calculations. *Journal of Alloys and Compounds*, **2017**, 690, 942-952	5.7	19
175	Generalized gradient calculations of structural, electronic and optical properties of MgxCd1□xO oxides. *Journal of Alloys and Compounds*, **2010**, 493, 212-218	5.7	19
174	Theoretical investigation of electronic structure and thermoelectric properties of MX2 (M=Zr, Hf; X=S, Se) van der Waals heterostructures. *Journal of Physics and Chemistry of Solids*, **2019**, 126, 304-309	3.9	19
173	Structural, optical, and electrical characteristics of AlN:Ho thin films irradiated with 700 keV protons. *Applied Surface Science*, **2015**, 357, 179-183	6.7	18
172	Detailed DFT studies of the band profiles and optical properties of antiperovskites SbNCa3 and BiNCa3. *Computational Materials Science*, **2014**, 85, 310-315	3.2	18
171	Theoretical studies of the osmium based perovskites AOsO3 (A=Ca, Sr and Ba). *Journal of Physics and Chemistry of Solids*, **2015**, 86, 114-121	3.9	17
170	Gain assisted multiple surperluminal regions via a Kerr nonlinearity in a double lambda-type atomic configuration. *Laser Physics*, **2014**, 24, 055401	1.2	17
169	Linear and nonlinear optical response of MgxZn1□xO: A density functional study. *Physica B: Condensed Matter*, **2011**, 406, 2632-2636	2.8	17
168	Influence of electric field on CO2 removal by P-doped C60-fullerene: A DFT study. *Chemical Physics Letters*, **2020**, 742, 137155	2.5	16
167	Synthesis, characterization, and biological study of some biologically potent schiff base transition metal complexes. *Russian Journal of Coordination Chemistry/Koordinatsionnaya Khimiya*, **2008**, 34, 678-682	1.6	16
166	Effects of cobalt substitution on the physical properties of the perovskite strontium ferrite. *Materials Chemistry and Physics*, **2017**, 196, 222-228	4.4	15
165	Coherent control of polarization state rotation via Doppler broadening and Kerr nonlinearity in a spinning fast light medium. *Laser Physics*, **2014**, 24, 115404	1.2	15
164	Thermoelectric properties of metallic antiperovskites AXD3 (A=Ge, Sn, Pb, Al, Zn, Ga; X=N, C; D=Ca, Fe, Co). *Electronic Materials Letters*, **2015**, 11, 466-480	2.9	15
163	First-Principles Study of Perovskite Molybdates AMoO3 (A = Ca, Sr, Ba). *Journal of Electronic Materials*, **2019**, 48, 1730-1739	1.9	15
162	Density functional theory study of emerging pollutants removal from water by covalent triazine based framework. *Journal of Molecular Liquids*, **2020**, 309, 113008	6	15
161	Optoelectronic properties of LixAxNbO3 (A=Na, K, Rb, Cs, Fr) crystals. *Physica B: Condensed Matter*, **2012**, 407, 368-377	2.8	14
160	Optoelectronic properties of KDP by first principle calculations. *International Journal of Quantum Chemistry*, **2013**, 113, 865-872	2.1	13

159	First principle studies of electronic and magnetic properties of Lanthanide-Gold (RAu) binary intermetallics. *Journal of Magnetism and Magnetic Materials*, **2017**, 422, 458-463	2.8	13
158	Comparison of the electronic band profiles and magneto-optic properties of cubic and orthorhombic SrTbO3. *Physica B: Condensed Matter*, **2013**, 423, 16-20	2.8	13
157	Photodetachment of H near a Hard Spherical Surface. *Chinese Physics Letters*, **2012**, 29, 013202	1.8	13
156	Structural, microwave permittivity, and complex impedance studies of cation (Cr, Bi, Al, In) substituted SrNi-X hexagonal nano-sized ferrites. *Ceramics International*, **2020**, 46, 1907-1915	5.1	13
155	Tunable surface plasmon polaritons at the surfaces of nanocomposite media. *Europhysics Letters*, **2018**, 122, 17001	1.6	13
154	First-principle studies of the optoelectronic properties of ASnF3 (A = Na, K, Rb and Cs). *International Journal of Modern Physics B*, **2017**, 31, 1750148	1.1	12
153	Electronic band structures of binary skutterudites. *Journal of Alloys and Compounds*, **2015**, 647, 364-369	5.7	12
152	Gray-box Soft Sensors in Process Industry: Current Practice, and Future Prospects in Era of Big Data. *Processes*, **2020**, 8, 243	2.9	12
151	Role of nitrogen vacancies in cerium doped aluminum nitride. *Journal of Magnetism and Magnetic Materials*, **2016**, 412, 49-54	2.8	12
150	Quasiparticle optoelectronic properties of pure and doped indium oxide. *Optical Materials*, **2012**, 34, 1406-1414	3.3	12
149	High-Performance Prediction of Molten Steel Temperature in Tundish through Gray-Box Model. *ISIJ International*, **2013**, 53, 76-80	1.7	12
148	Magneto-electronic studies of anti-perovskites NiNMn3 and ZnNMn3. *Computational Materials Science*, **2014**, 81, 141-145	3.2	12
147	Optoelectronic Response of GeZn 2 O 4 through the Modified Becke Johnson Potential. *Chinese Physics Letters*, **2012**, 29, 097102	1.8	12
146	Theoretical investigation of half-metallicity in Co/Ni substituted AlN. *International Journal of Quantum Chemistry*, **2012**, 112, 882-888	2.1	12
145	Ab initio studies of electric field gradients and magnetic properties of uranium dipnicties. *RSC Advances*, **2015**, 5, 37592-37602	3.7	11
144	van der Waals heterostructures based on MSSe (M = Mo, W) and graphene-like GaN: enhanced optoelectronic and photocatalytic properties for water splitting. *Physical Chemistry Chemical Physics*, **2020**, 22, 20704-20711	3.6	11
143	Structural and magnetic properties of TlTF3 (T=Fe, Co and Ni) by hybrid functional theory. *Journal of Magnetism and Magnetic Materials*, **2015**, 388, 143-149	2.8	10
142	Tunable relativistic quasiparticle electronic and excitonic behavior of the FAPb(IBr) alloy. *Physical Chemistry Chemical Physics*, **2020**, 22, 11943-11955	3.6	10

141	Control of Group Velocity via Spontaneous Generated Coherence and Kerr Nonlinearity. *Communications in Theoretical Physics*, **2014**, 62, 410-416	2.4	10
140	Deep ultraviolet photopumped stimulated emission from partially relaxed AlGaN multiple quantum well heterostructures grown on sapphire substrates. *Journal of Vacuum Science and Technology B:Nanotechnology and Microelectronics*, **2014**, 32, 061204	1.3	10
139	Pressure driven spin crossover and isostructural phase transition in LaFeO3. *Journal of Applied Physics*, **2013**, 114, 243712	2.5	10
138	First principle optoelectronic studies of visible light sensitive CZT. *Superlattices and Microstructures*, **2013**, 63, 91-99	2.8	10
137	Electronic band structure of LaCoO3/Y/Mn compounds. *Physica B: Condensed Matter*, **2013**, 410, 112-119	2.8	10
136	Control of slow-to-fast light and single-to-double optomechanically induced transparency in a compound resonator system: A theoretical approach. *Europhysics Letters*, **2017**, 120, 24001	1.6	10
135	Optical properties of ideal □Al2O3 and with oxygen point defects: an ab initio study. *RSC Advances*, **2015**, 5, 55088-55099	3.7	10
134	Effect of size reduction on the electronic and ferromagnetic properties of the In2O3 nanoparticles. *Journal of Nanoparticle Research*, **2012**, 14, 1	2.3	10
133	Ultraviolet spectroscopy of Pr+3 and its use in making ultraviolet filters. *Current Applied Physics*, **2009**, 9, 234-237	2.6	10
132	Comparative study of thermoelectric properties of Co based filled antimonide skutterudites with and without SOC effect. *Computational Materials Science*, **2017**, 131, 308-314	3.2	9
131	Effects of dangling bonds and diameter on the electronic and optical properties of InAs nanowires. *RSC Advances*, **2015**, 5, 23320-23325	3.7	9
130	A first-principles study of electronic structure and photocatalytic performance of GaN-MX (M = Mo, W; X= S, Se) van der Waals heterostructures.. *RSC Advances*, **2020**, 10, 24683-24690	3.7	9
129	Pressure dependency of localization degree in heavy fermion CeIn3: A density functional theory analysis. *Scientific Reports*, **2016**, 6, 31734	4.9	9
128	Robust Half-Metallicity and Magnetic Properties of Cubic Perovskite CaFeO 3. *Chinese Physics Letters*, **2013**, 30, 047504	1.8	9
127	Effects of chemical potential on the thermoelectric performance of alkaline-earth based skutterudites (AFe4Sb12, A Ca, Sr and Ba). *Journal of Alloys and Compounds*, **2017**, 694, 253-260	5.7	9
126	DFT-mBJ Studies of the Band Structures of the II-VI Semiconductors. *Materials Today: Proceedings*, **2015**, 2, 5122-5127	1.4	9
125	Robust half-metallicity of AlCoN and AlNiN. *International Journal of Quantum Chemistry*, **2012**, 112, 2668-2674	2.2	9
124	Comparison of band profiles and magnetic properties of the different phases of BaTbO3. *Computational Materials Science*, **2013**, 67, 151-155	3.2	9

123	Classification of partially reflecting surfaces using photodetached electron spectrum. *International Journal of Quantum Chemistry*, **2011**, 111, 4067-4071	2.1	9
122	Electron penetration depth in amorphous AlN exploiting the luminescence of AlN:Tm/AlN:Ho bilayers. *Current Applied Physics*, **2009**, 9, 417-421	2.6	9
121	Interferences in photodetachment of a triatomic negative ion. *Applied Physics Letters*, **2009**, 94, 041125	3.4	9
120	Spectroscopy of gadolinium ion and disadvantages of gadolinium impurity in tissue compensators and collimators, used in radiation treatment planning. *Spectroscopy*, **2007**, 21, 205-210		9
119	Influence of Cr and Zn substitution on structural, magnetic and dielectric properties of Sr2-xZnxNi2Fe28-yCryO46 X-type hexagonal ferrite. *Solid State Sciences*, **2020**, 100, 106090	3.4	9
118	First-principles study of BiFeO3 and BaTiO3 in tetragonal structure. *International Journal of Modern Physics B*, **2019**, 33, 1950231	1.1	8
117	Prediction of Molten Steel Temperature in Steel Making Process with Uncertainty by Integrating Gray-Box Model and Bootstrap Filter. *Journal of Chemical Engineering of Japan*, **2014**, 47, 827-834	0.8	8
116	Structural, electronical and thermoelectric properties of CdGa2S4 compound under high pressures by mBJ approach. *Journal of Materials Science: Materials in Electronics*, **2017**, 28, 16476-16483	2.1	8
115	Energy level splitting and luminescence enhancement in AlN:Er by an external magnetic field. *Optical Materials*, **2015**, 46, 601-604	3.3	8
114	Nanocrystals formation and intense green emission in thermally annealed AlN:Ho films for microlaser cavities and photonic applications. *Journal of Applied Physics*, **2010**, 108, 043528	2.5	8
113	First-principles study of structural, electronic, magnetic and thermoelectric properties of the cubic mono-pnictides of thorium Th Pn (Pn = Sb and Bi). *Computational Condensed Matter*, **2017**, 13, 111-119	1.7	7
112	Temporal characteristics of aerosol optical properties over the glacier region of northern Pakistan. *Journal of Atmospheric and Solar-Terrestrial Physics*, **2019**, 186, 35-46	2	7
111	Mechanical properties and variation in SOC going from La to Nd in intermetallic RIn3 and RSn3 (R = La, Ce, Pr, Nd). *RSC Advances*, **2015**, 5, 39416-39423	3.7	7
110	Effects of Ni Substitution on the Electronic Structure and Magnetic Properties of Perovskite SrFeO3. *Journal of Electronic Materials*, **2020**, 49, 3780-3790	1.9	7
109	First principle studies of structural, magnetic and elastic properties of orthorhombic rare-earth diaurides intermetallics RAu2 (R=La, Ce, Pr and Eu). *Materials Chemistry and Physics*, **2018**, 212, 44-50	4.4	7
108	DFT study on thermo-elastic properties of Ru2FeZ (Z = Si, Ge, Sn) Heusler alloys. *International Journal of Modern Physics B*, **2018**, 32, 1850045	1.1	7
107	Unusual refraction and Fizeau effect for a linearly polarized pulse in rotary chiral media. *Journal of the Optical Society of America B: Optical Physics*, **2018**, 35, 1817	1.7	7
106	Density functional studies of magneto-optic properties of CdCoS. *Journal of Magnetism and Magnetic Materials*, **2014**, 351, 60-64	2.8	7

105	Pseudomorphic AlxGa1-xN MQW based deep ultraviolet light emitting diodes over sapphire. *Physica Status Solidi C: Current Topics in Solid State Physics*, **2014**, 11, 798-801		7
104	The effect of Kerr nonlinearity and Doppler broadening on slow light propagation. *Laser Physics*, **2014**, 24, 025201	1.2	7
103	Control of Wave Propagation and Effect of Kerr Nonlinearity on Group Index. *Communications in Theoretical Physics*, **2013**, 60, 87-92	2.4	7
102	125 Te NMR shielding and optoelectronic spectra in XTe 3 O 8 (X□=□Ti, Zr, Sn and Hf) compounds: Ab initio calculations. *Journal of Molecular Structure*, **2017**, 1148, 223-230	3.4	7
101	First principle study of band gap nature, spontaneous polarization, hyperfine field and electric field gradient of desirable multiferroic bismuth ferrite (BiFeO3). *Journal of Physics and Chemistry of Solids*, **2021**, 148, 109737	3.9	7
100	Selective adsorption of CO from gas mixture by P-decorated CN fullerene assisted by an electric field: A DFT approach. *Journal of Molecular Graphics and Modelling*, **2021**, 103, 107806	2.8	7
99	Silicon carbide and III-Nitrides nanosheets: Promising anodes for Mg-ion batteries. *Materials Chemistry and Physics*, **2021**, 257, 123785	4.4	7
98	Theoretical investigation of thermoelectric and elastic properties of intermetallic compounds ScTM (TM = Cu, Ag, Au and Pd). *International Journal of Modern Physics B*, **2018**, 32, 1850004	1.1	6
97	Cross-Kerr nonlinearity in the surface plasmon polariton waves generated at the interface of graphene and gain medium. *Europhysics Letters*, **2018**, 122, 57003	1.6	6
96	Van der Waals heterostructures of blue phosphorene and scandium-based MXenes monolayers. *Journal of Applied Physics*, **2019**, 126, 143101	2.5	6
95	Investigation of the optical properties of P, As and Sb incorporated AlGaX alloys using full potential linearized augmented plane wave method. *Computer Physics Communications*, **2014**, 185, 2829-2833	4.2	6
94	Temporal cloak via Doppler broadening. *Laser Physics*, **2015**, 25, 065405	1.2	6
93	Luminescence from Cr+3-doped AlN films deposited on optical fiber and silicon substrates for use as waveguides and laser cavities. *Applied Optics*, **2010**, 49, 653-7	0.2	6
92	Investigation of Linear Tetra-Atomic Negative Ion by Photodetached-Electron Spectra. *Chinese Physics Letters*, **2011**, 28, 083301	1.8	6
91	Interferences in Photodetached Electron Spectra from a Linear Tetra-Atomic Negative Ion. *Chinese Physics Letters*, **2011**, 28, 063301	1.8	6
90	Electronic structure of the LiAA?O6 (A□=□Nb, Ta, and A?□=□W, Mo) ceramics by modified Becke-Johnson potential. *Optical Materials*, **2016**, 58, 466-475	3.3	6
89	First-principles studies of pure and fluorine substituted alanines. *International Journal of Modern Physics B*, **2016**, 30, 1650079	1.1	6
88	Elastic and Optoelectronic Properties of Cs2NaMCl6 (M = In, Tl, Sb, Bi). *Journal of Electronic Materials*, **2021**, 50, 456-466	1.9	6

87	Removal of azo dye from aqueous solution by a low-cost activated carbon prepared from coal: adsorption kinetics, isotherms study, and DFT simulation. *Environmental Science and Pollution Research*, **2021**, 28, 10234-10247	5.1	6
86	Effect of strain on structural and electronic properties, and thermoelectric response of MXY (M=Zr, Hf and Pt; X/Y=S, Se) vdW heterostructures; A first principles study. *Journal of Solid State Chemistry*, **2021**, 299, 122189	3.3	6
85	I NMR calculations in binary metal iodides by PBE-GGA, YS-PBE0 and mBJ exchange correlation potentials. *Solid State Nuclear Magnetic Resonance*, **2017**, 82-83, 10-15	3.1	5
84	Spatio-temporal variations of absorbing aerosols and their relationship with meteorology over four high altitude sites in glaciated region of Pakistan. *Journal of Atmospheric and Solar-Terrestrial Physics*, **2019**, 190, 84-95	2	5
83	Magneto-electronic studies of the inverse-perovskite (Eu3O)In. *Journal of Magnetism and Magnetic Materials*, **2015**, 381, 34-40	2.8	5
82	Irradiation effects on Nd and W doped Aluminum Nitride thin films. *Physica B: Condensed Matter*, **2020**, 586, 412086	2.8	5
81	Black Carbon aerosol characteristics and radiative forcing over the high altitude glacier region of Himalaya-Karakorum-Hindukush. *Atmospheric Environment*, **2020**, 238, 117711	5.3	5
80	High-Temperature Operation of AlxGa1□N (x > 0.4) Channel Metal Oxide Semiconductor Heterostructure Field Effect Transistors with High-k Atomic Layer Deposited Gate Oxides. *Physica Status Solidi (A) Applications and Materials Science*, **2020**, 217, 1900802	1.6	5
79	Conductivity dependent surface plasmon polariton propagation. *Laser Physics*, **2016**, 26, 095204	1.2	5
78	Superluminal propagation in a poly-chromatically driven gain assisted four-level N-type atomic system. *Physica Scripta*, **2013**, 88, 045402	2.6	5
77	Electron correlation and spin-orbit coupling effects in scandium intermetallic compounds ScTM (TM = Co, Rh, Ir, Ni, Pd, Pt, Cu, Ag and Au). *International Journal of Modern Physics B*, **2017**, 31, 1750263	1.1	5
76	Dimensions and Analysis of Uncertainty in Industrial Modeling Process. *Journal of Chemical Engineering of Japan*, **2018**, 51, 533-543	0.8	5
75	Role of the Crystal Lattice Constants and Band Structures in the Optoelectronic Spectra of CdGa2S4 by DFT Approaches. *Zeitschrift Fur Anorganische Und Allgemeine Chemie*, **2017**, 643, 839-849	1.3	4
74	First principles studies of CsLnCdTe3 (Ln = Gd□Tm) for green energy resources. *Computational Condensed Matter*, **2019**, 21, e00427	1.7	4
73	A computational study on the characteristics of open-shell H-bonding interaction between carbamic acid (NHCOOH) and HO, HOS or HSO radicals. *Journal of Molecular Modeling*, **2019**, 25, 189	2	4
72	Physical properties and possible applications of gold-based rare earth intermetallics (R-Au): A review. *Journal of Magnetism and Magnetic Materials*, **2019**, 490, 165477	2.8	4
71	Enhanced and highly tunable Goos-H□chan shifts at a nanocomposite-graphene interface. *Applied Physics Letters*, **2019**, 114, 161902	3.4	4
70	Effects of A-Site cation on the Physical Properties of Quaternary Perovskites AMn3V4O12 (A= Ca, Ce and Sm). *Materials Chemistry and Physics*, **2020**, 254, 123229	4.4	4

69	DFT and post-DFT studies of metallic MXY3-type compounds for low temperature TE applications. *Solid State Communications*, **2016**, 243, 28-35	1.6	4
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