Imad Khan

List of Publications by Year
in descending order

51 papers	1,102 citations	394421 19 h-index	434195 31 g-index
51 all docs	51 docs citations	51 times ranked	689 citing authors

#	Article	IF	Citations
1	First-principles prediction of the ground-state crystal structure of double-perovskite halides Cs2AgCrX6 (X = Cl, Br, and I). Journal of Physics and Chemistry of Solids, 2022, 160, 110302.	4.0	64
2	First principle studies of structural, elastic, electronic and optical properties of Zn-chalcogenides under pressure. Journal of Semiconductors, 2014, 35, 072001.	3.7	58
3	Thermoelectric studies of IVâ€“VI semiconductors for renewable energy resources. Materials Science in Semiconductor Processing, 2016, 48, 85-94.	4.0	58
4	Electronic structure of cubic perovskite SnTaO3. Intermetallics, 2012, 31, 287-291.	3.9	55
5	Electronic Band Structures of the Highly Desirable IIIâ€“V Semiconductors: TB-mBJ DFT Studies. Journal of Electronic Materials, 2016, 45, 3314-3323.	2.2	54
6	Conversion of optically isotropic to anisotropic CdSxSe1â^'x (0â©½xâ©½1) alloy with S concentration. Computational Materials Science, 2013, 77, 145-152.	3.0	48
7	Effect of phase transition on the optoelectronic properties of Zn1â^'xMgxS. Journal of Applied Physics, 2012, 112, .	2.5	45
8	Structural and optoelectronic properties of the zinc titanate perovskite and spinel by modified Beckeâ€“Johnson potential. Physica B: Condensed Matter, 2013, 420, 54-57.	2.7	44
9	Electronic and optical properties of mixed Be-chalcogenides. Journal of Physics and Chemistry of Solids, 2013, 74, 181-188.	4.0	42
10	First-principles study of BiFeO₃and BaTiO₃in tetragonal structure. International Journal of Modern Physics B, 2019, 33, 1950231.	2.0	40
11	Optoelectronic and elastic properties of metal halides double perovskites Cs2InBiX6 (X = F, Cl, Br, I). Chinese Optics Letters, 2021, 19, 030004.	2.9	39
12	Theoretical studies of the paramagnetic perovskites MTaO3 (MÂ=ÂCa, Sr and Ba). Materials Chemistry and Physics, 2015, 162, 308-315.	4.0	38
13	Elastic and Optoelectronic Properties of Cs2NaMCl6 (M = In, Tl, Sb, Bi). Journal of Electronic Materials, 2021, 50, 456-466.	2.2	33
14	Structural and optoelectronic properties of Mg substituted ZTe (Z=Zn, Cd and Hg). Journal of Physics and Chemistry of Solids, 2015, 83, 75-84.	4.0	32
15	Transition from optically inactive to active Mg-chalcogenides: A first principle study. Computational Materials Science, 2012, 61, 278-282.	3.0	27
16	Effects of cobalt substitution on the physical properties of the perovskite strontium ferrite. Materials Chemistry and Physics, 2017, 196, 222-228.	4.0	26
17	Theoretical studies of the band structure and optoelectronic properties of ZnO_xS_{1â^'x}. International Journal of Quantum Chemistry, 2013, 113, 1285-1292.	2.0	25
18	First-Principles Study of Perovskite Molybdates AMoO3 (Aâ€‰=â€‰Ca, Sr, Ba). Journal of Electronic Materials, 2019, 48, 1730-1739.	2.2	23

#	Article	IF	Citations
19	Electronic structure and magnetic properties of the perovskites SrTMO3 (TM = Mn, Fe, Co, Tc, Ru, Rh,) Tj ETQq1 1 0.784314 rgBT /Over	2.7	21
20	Effects of Ni Substitution on the Electronic Structure and Magnetic Properties of Perovskite SrFeO3. Journal of Electronic Materials, 2020, 49, 3780-3790.	2.2	19
21	First-principle studies of the optoelectronic properties of ASnF₃ (A = Na, K, Rb and Cs). International Journal of Modern Physics B, 2017, 31, 1750148.	2.0	18
22	DFT-mBJ Studies of the Band Structures of the II-VI Semiconductors. Materials Today: Proceedings, 2015, 2, 5122-5127.	1.8	17
23	First-principles study of the structural and optoelectronic properties of ANbO3 (A = Na, K and Rb) in four crystal phases. Materials Science in Semiconductor Processing, 2022, 139, 106364.	4.0	17
24	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.	2.3	16
25	Theoretical Investigations of Quaternary Semiconductors CsInCdTe3 (Lnâ€‰=â€‰La, Pr, Nd and Sm). Journal of Electronic Materials, 2020, 49, 3357-3366.	2.2	16
26	Robust Half-Metallicity and Magnetic Properties of Cubic Perovskite CaFeO 3. Chinese Physics Letters, 2013, 30, 047504.	3.3	15
27	First principle optoelectronic studies of visible light sensitive CZT. Superlattices and Microstructures, 2013, 63, 91-99.	3.1	15
28	Comparison of the electronic band profiles and magneto-optic properties of cubic and orthorhombic SrTbO3. Physica B: Condensed Matter, 2013, 423, 16-20.	2.7	15
29	Electronic structure, optical and magnetic properties of double Perovskites La2MTiO6 (M = Co, Ni, Cu) Tj ETQq1 1 0.784314 rgBT /Over	4.0	15
30	Magneto-electronic studies of anti-perovskites NiNMn3 and ZnNMn3. Computational Materials Science, 2014, 81, 141-145.	3.0	14
31	Effects of A-Site cation on the Physical Properties of Quaternary Perovskites AMn3V4O12 (A= Ca, Ce) Tj ETQq1 1 0.784314 rgBT /Over	4.0	14
32	Electronic band structures of binary skutterudites. Journal of Alloys and Compounds, 2015, 647, 364-369.	5.5	13
33	Electronic Structure, Mechanical and Magnetic Properties of the Quaternary Perovskites CaA3V4O12 (Aâ€‰=â€‰Mn, Fe, Co, Ni and Cu). Journal of Electronic Materials, 2020, 49, 1230-1242.	2.2	12
34	Electronic band structure of LaCoO3/Y/Mn compounds. Physica B: Condensed Matter, 2013, 410, 112-119.	2.7	11
35	Comparative study of thermoelectric properties of Co based filled antimonide skutterudites with and without SOC effect. Computational Materials Science, 2017, 131, 308-314.	3.0	11
36	Spin-orbit coupling effect on the optoelectronic and thermoelectric properties of the perovskites A3SnO (A = Ca, Sr and Ba). Materials Science in Semiconductor Processing, 2021, 132, 105905.	4.0	11

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37	Density functional studies of magneto-optic properties of CdCoS. Journal of Magnetism and Magnetic Materials, 2014, 351, 60-64.	2.3	10
38	Electronic structure of the LiAAâ€²O6 (AÂ=ÂNb, Ta, and Aâ€²Â=ÂW, Mo) ceramics by modified Becke-Johnson potential. Optical Materials, 2016, 58, 466-475.	3.6	10
39	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.	5.5	10
40	First principles studies of CsLnCdTe3 (LnÂ= Gdâ^'Tm) for green energy resources. Computational Condensed Matter, 2019, 21, e00427.	2.1	7
41	The effect of potassium insertion on optoelectronic properties of cadmium chalcogenides. Materials Science in Semiconductor Processing, 2021, 122, 105466.	4.0	7
42	First-principle studies of the ternary palladates CaPd3O4 and SrPd3O4. Bulletin of Materials Science, 2016, 39, 1861-1870.	1.7	6
43	First-principles studies of pure and fluorine substituted alanines. International Journal of Modern Physics B, 2016, 30, 1650079.	2.0	6
44	Magneto-electronic studies of the inverse-perovskite (Eu3O)In. Journal of Magnetism and Magnetic Materials, 2015, 381, 34-40.	2.3	5
45	Structural, Mechanical and Optoelectronic Properties of Y2M2O7 (M = Ti, V and Nb) Pyrochlores: A First Principles Study. Journal of Electronic Materials, 2017, 46, 4640-4648.	2.2	5
46	First-Principles Study of Electronic Structure, Mechanical, and Thermoelectric Properties of Ternary Palladates CdPd3O4 and TlPd3O4. Journal of Electronic Materials, 2018, 47, 1871-1880.	2.2	4
47	Theoretical studies of the electronic structure and magnetic properties of aluminum-rich intermetallic alloy Al13Fe₄. International Journal of Modern Physics B, 2018, 32, 1850201.	2.0	4
48	Structural and optoelectronic properties of CsLnZnTe3 (LnÂ= La, Pr, Nd and Sm). Journal of Rare Earths, 2023, 41, 388-396.	4.8	4
49	Structural, Mechanical and Magneto-Electronic Properties of the Ternary Sodium Palladium and Platinum Oxides. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 2015, 70, 815-822.	1.5	1
50	The Influence of Oxygen Substitution on the Optoelectronic Properties of ZnTe. Journal of Chemistry, 2016, 2016, 1-8.	1.9	1
51	Electronic structure and magnetic properties of the Mg-rich intermetallic NdNiMg5 by hybrid density functional theory. Intermetallics, 2020, 127, 106969.	3.9	1