

# Zahid Ali

## List of Publications by Year in descending order

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papers

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#	ARTICLE	IF	CITATIONS
1	Thermoelectric studies of IV-VI semiconductors for renewable energy resources. <i>Materials Science in Semiconductor Processing</i> , 2016, 48, 85-94.	4.0	58
2	Electronic structure of cubic perovskite SnTaO <sub>3</sub> . <i>Intermetallics</i> , 2012, 31, 287-291.	3.9	55
3	Theoretical studies of structural and magnetic properties of cubic perovskites PrCoO <sub>3</sub> and NdCoO <sub>3</sub> . <i>Physica B: Condensed Matter</i> , 2011, 406, 3800-3804.	2.7	48
4	Conversion of optically isotropic to anisotropic Cd <sub>x</sub> Se <sub>1-x</sub> (0 ≤ x ≤ 1) alloy with S concentration. <i>Computational Materials Science</i> , 2013, 77, 145-152.	3.0	48
5	Structural and optoelectronic properties of the zinc titanate perovskite and spinel by modified Becke-Johnson potential. <i>Physica B: Condensed Matter</i> , 2013, 420, 54-57.	2.7	44
6	GGA+U studies of the cubic perovskites BaMO <sub>3</sub> (M=Pr, Th and U). <i>Physica B: Condensed Matter</i> , 2013, 410, 217-221.	2.7	41
7	First-principles study of BiFeO <sub>3</sub> and BaTiO <sub>3</sub> in tetragonal structure. <i>International Journal of Modern Physics B</i> , 2019, 33, 1950231.	2.0	40
8	Theoretical studies of the paramagnetic perovskites MTaO <sub>3</sub> (M=Ca, Sr and Ba). <i>Materials Chemistry and Physics</i> , 2015, 162, 308-315.	4.0	38
9	Bandgap engineering of Cd <sub>1-x</sub> Sr <sub>x</sub> O. <i>Physica B: Condensed Matter</i> , 2011, 406, 2509-2514.	2.7	33
10	Elastic and Optoelectronic Properties of Cs <sub>2</sub> NaMCl <sub>6</sub> (M = In, Tl, Sb, Bi). <i>Journal of Electronic Materials</i> , 2021, 50, 456-466.	2.2	33
11	Structural and optoelectronic properties of Mg substituted ZTe (Z=Zn, Cd and Hg). <i>Journal of Physics and Chemistry of Solids</i> , 2015, 83, 75-84.	4.0	32
12	Band Profile Comparison of the Cubic Perovskites CaCoO <sub>3</sub> and SrCoO <sub>3</sub> . <i>Journal of Electronic Materials</i> , 2013, 42, 438-444.	2.2	27
13	Effects of cobalt substitution on the physical properties of the perovskite strontium ferrite. <i>Materials Chemistry and Physics</i> , 2017, 196, 222-228.	4.0	26
14	First-Principles Study of Perovskite Molybdates AMoO <sub>3</sub> (A=Ca, Sr, Ba). <i>Journal of Electronic Materials</i> , 2019, 48, 1730-1739.	2.2	23
15	Theoretical studies of the osmium based perovskites AOsO <sub>3</sub> (A=Ca, Sr and Ba). <i>Journal of Physics and Chemistry of Solids</i> , 2015, 86, 114-121.	4.0	22
16	Electronic structure and magnetic properties of the perovskites SrTMO <sub>3</sub> (TM = Mn, Fe, Co, Tc, Ru, Rh). <i>Journal of Electronic Materials</i> , 2019, 48, 1730-1739.	2.7	21
17	Effects of Ni Substitution on the Electronic Structure and Magnetic Properties of Perovskite SrFeO <sub>3</sub> . <i>Journal of Electronic Materials</i> , 2020, 49, 3780-3790.	2.2	19
18	First-principle studies of the optoelectronic properties of ASnF <sub>3</sub> (A = Na, K, Rb and Cs). <i>International Journal of Modern Physics B</i> , 2017, 31, 1750148.	2.0	18

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19	First-principles study of the structural and optoelectronic properties of ANbO <sub>3</sub> (A = Na, K and Rb) in four crystal phases. <i>Materials Science in Semiconductor Processing</i> , 2022, 139, 106364.	4.0	17
20	Structural and magnetic properties of TlTf <sub>3</sub> (T=Fe, Co and Ni) by hybrid functional theory. <i>Journal of Magnetism and Magnetic Materials</i> , 2015, 388, 143-149.	2.3	16
21	Theoretical Investigations of Quaternary Semiconductors CsInCdTe <sub>3</sub> (Ln=La, Pr, Nd and Sm). <i>Journal of Electronic Materials</i> , 2020, 49, 3357-3366.	2.2	16
22	Robust Half-Metallicity and Magnetic Properties of Cubic Perovskite CaFeO <sub>3</sub> . <i>Chinese Physics Letters</i> , 2013, 30, 047504.	3.3	15
23	First principle optoelectronic studies of visible light sensitive CZT. <i>Superlattices and Microstructures</i> , 2013, 63, 91-99.	3.1	15
24	Comparison of the electronic band profiles and magneto-optic properties of cubic and orthorhombic SrTbO <sub>3</sub> . <i>Physica B: Condensed Matter</i> , 2013, 423, 16-20.	2.7	15
25	Electronic structure, optical and magnetic properties of double Perovskites La <sub>2</sub> MTiO <sub>6</sub> (M = Co, Ni, Cu) <i>TJ ETQq1 1 0.784314 rgBT /Over</i>	4.0	15
26	Magneto-electronic studies of anti-perovskites NiNMn <sub>3</sub> and ZnNMn <sub>3</sub> . <i>Computational Materials Science</i> , 2014, 81, 141-145.	3.0	14
27	Effects of A-Site cation on the Physical Properties of Quaternary Perovskites AMn <sub>3</sub> V <sub>4</sub> O <sub>12</sub> (A= Ca, Ce) <i>TJ ETQq1 1 0.784314 rgBT /Over</i>	4.0	14
28	First principle studies of electronic and magnetic properties of Lanthanide-Gold (RAu) binary intermetallics. <i>Journal of Magnetism and Magnetic Materials</i> , 2017, 422, 458-463.	2.3	13
29	Electronic Structure, Mechanical and Magnetic Properties of the Quaternary Perovskites CaA <sub>3</sub> V <sub>4</sub> O <sub>12</sub> (A=Mn, Fe, Co, Ni and Cu). <i>Journal of Electronic Materials</i> , 2020, 49, 1230-1242.	2.2	12
30	First principle studies of structural, magnetic and elastic properties of orthorhombic rare-earth diaurides intermetallics RAu <sub>2</sub> (R=La, Ce, Pr and Eu). <i>Materials Chemistry and Physics</i> , 2018, 212, 44-50.	4.0	11
31	Spin-orbit coupling effect on the optoelectronic and thermoelectric properties of the perovskites A <sub>3</sub> SnO (A = Ca, Sr and Ba). <i>Materials Science in Semiconductor Processing</i> , 2021, 132, 105905.	4.0	11
32	Density functional studies of magneto-optic properties of CdCoS. <i>Journal of Magnetism and Magnetic Materials</i> , 2014, 351, 60-64.	2.3	10
33	Electronic structure of the LiAA <sub>2</sub> O <sub>6</sub> (A= Nb, Ta, and A <sub>2</sub> = W, Mo) ceramics by modified Becke-Johnson potential. <i>Optical Materials</i> , 2016, 58, 466-475.	3.6	10
34	<i>i&gt;n&lt;/i&gt;-Type narrow band gap A<sub>3</sub>InAs<sub>3</sub> (A= Sr and Eu) Zintl phase semiconductors for optoelectronic and thermoelectric applications. <i>Journal of Taibah University for Science</i>, 2022, 16, 660-669.</i>	2.5	10
35	Comparison of band profiles and magnetic properties of the different phases of BaTbO <sub>3</sub> . <i>Computational Materials Science</i> , 2013, 67, 151-155.	3.0	9
36	New anti-ferromagnetic tri-transition quaternary perovskites for magnetic cloaking and spintronic applications. <i>Materials Chemistry and Physics</i> , 2022, 282, 125915.	4.0	9

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37	First principle study of opto-electronic and thermoelectric properties of Zintl Phase $X\text{In}_2\text{Z}_2$ ( $X = \text{Ca, Sr}$ )	2.3	8
38	First principles studies of $\text{CsLnCdTe}_3$ ( $\text{Ln} = \text{Gd} \sim \text{Tm}$ ) for green energy resources. Computational Condensed Matter, 2019, 21, e00427.	2.1	7
39	Structural, electronic, optical and thermoelectric properties in the phases of $\text{AgTaO}_3$ . Materials Science in Semiconductor Processing, 2021, 122, 105467.	4.0	7
40	The effect of potassium insertion on optoelectronic properties of cadmium chalcogenides. Materials Science in Semiconductor Processing, 2021, 122, 105466.	4.0	7
41	Hybrid DFT study of structural, electronic, magnetic and elastic properties of laves phase binary intermetallics $\text{RFe}_2$ ( $\text{R} = \text{La, Ce, Pr and Nd}$ ). Journal of Rare Earths, 2023, 41, 1367-1375.	4.8	7
42	First-principle studies of the ternary palladates $\text{CaPd}_3\text{O}_4$ and $\text{SrPd}_3\text{O}_4$ . 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	Structural, optoelectronic and elastic properties of quaternary perovskites $\text{CaPd}_3\text{B}_4\text{O}_{12}$ ( $\text{B} = \text{Ti, V}$ ). International Journal of Modern Physics B, 2019, 33, 1950212.	2.0	6
45	Magneto-electronic studies of the inverse-perovskite $(\text{Eu}_3\text{O})\text{In}$ . Journal of Magnetism and Magnetic Materials, 2015, 381, 34-40.	2.3	5
46	Structural, Mechanical and Optoelectronic Properties of $\text{Y}_2\text{M}_2\text{O}_7$ ( $\text{M} = \text{Ti, V and Nb}$ ) Pyrochlores: A First Principles Study. Journal of Electronic Materials, 2017, 46, 4640-4648.	2.2	5
47	Electron correlation and spin-orbit coupling effects in scandium intermetallic compounds $\text{ScTM}$ ( $\text{TM}$ )	2.0	5
48	Electronic structure and magnetic properties of the quaternary perovskites $\text{LnMn}_3\text{V}_4\text{O}_{12}$ ( $\text{Ln} = \text{La, Nd and Gd}$ ). Philosophical Magazine, 2020, 100, 2386-2401.	1.6	5
49	First-Principles Study of Electronic Structure, Mechanical, and Thermoelectric Properties of Ternary Palladates $\text{CdPd}_3\text{O}_4$ and $\text{TlPd}_3\text{O}_4$ . Journal of Electronic Materials, 2018, 47, 1871-1880.	2.2	4
50	Theoretical studies of the electronic structure and magnetic properties of aluminum-rich intermetallic alloy $\text{Al}_3\text{Fe}_4$ . International Journal of Modern Physics B, 2018, 32, 1850201.	2.0	4
51	Structural and optoelectronic properties of $\text{CsLnZnTe}_3$ ( $\text{Ln} = \text{La, Pr, Nd and Sm}$ ). Journal of Rare Earths, 2023, 41, 388-396.	4.8	4
52	HKUST-1 Supported on Zirconium Phosphate as an Efficient Catalyst for Solvent Free Oxidation of Cyclohexene: DFT Study. Catalysts, 2018, 8, 546.	3.5	3
53	Structural, Electronic, Elastic and Magnetic Properties of $\text{Ln}_3\text{QIn}$ ( $\text{Ln} = \text{Ce, Pr and Nd}$ ; $\text{Q} = \text{C and N}$ ) anti-perovskites. Journal of Electronic Materials, 2022, 51, 2819-2827.	2.2	3
54	Electronic structure, elastic and magnetic properties of the binary intermetallics $\text{RFe}_2$ ( $\text{R} = \text{Eu, Gd and}$ )	2.5	3

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55	Optoelectronic, elastic and thermoelectric properties of the perovskites (Sr <sub>3</sub> N)Sb and (Sr <sub>3</sub> N)Bi. Materials Science in Semiconductor Processing, 2022, 147, 106734.	4.0	2
56	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
57	The Influence of Oxygen Substitution on the Optoelectronic Properties of ZnTe. Journal of Chemistry, 2016, 2016, 1-8.	1.9	1
58	Electronic structure and magnetic properties of the Mg-rich intermetallic NdNiMg <sub>5</sub> by hybrid density functional theory. Intermetallics, 2020, 127, 106969.	3.9	1
59	Optoelectronic properties of the double perovskites Ba <sub>2</sub> MM <sup>2+</sup> O <sub>6</sub> (M= Sc, Y, La; M <sup>2+</sup> = Nb, Ta) by modified Becke-Johnson potential. , 2020, , .		0