M A Ali

List of Publications by Year in Descending Order

49 papers	839 citations	19 h-index	27 g-index
49 ext. papers	1,111 ext. citations	2.7 avg, IF	4.99 L-index

#	Paper	IF	Citations
49	DFT insights into the new Hf-based chalcogenide MAX phase Hf2SeC. *Vacuum*, **2022**, 201, 111072	3.7	2
48	Newly Synthesized Three-Dimensional Boron-Rich Chalcogenides BX (X = S and Se): Theoretical Characterization of the Physical Properties for Optoelectronic and Mechanical Applications.. *ACS Omega*, **2021**, 6, 33899-33913	3.9	2
47	Mechanical, optical and high-temperature magnetic properties of Sn-substituted Mg□n ferrites. *Phase Transitions*, **2021**, 94, 23-36	1.3	
46	Physical properties of new MAX phase borides M2SB (M = Zr, Hf and Nb) in comparison with conventional MAX phase carbides M2SC (M = Zr, Hf and Nb): Comprehensive insights. *Journal of Materials Research and Technology*, **2021**, 11, 1000-1018	5.5	21
45	Influence of Se doping on recently synthesized NaInS2-xSex solid solutions for potential thermo-mechanical applications studied via first-principles method. *Materials Today Communications*, **2021**, 26, 101988	2.5	5
44	Impact of V substitution on the physical properties of Ni□nCo ferrites: structural, magnetic, dielectric and electrical properties. *Materials Research Express*, **2021**, 8, 046102	1.7	1
43	DFT insights into new B-containing 212 MAX phases: Hf2AB2 (A = In, Sn). *Journal of Alloys and Compounds*, **2021**, 860, 158408	5.7	14
42	Impact of Sn4+ substitution in Mg□n ferrites: Deciphering the structural, morphological, dielectric, electrical and magnetic properties. *Materials Chemistry and Physics*, **2021**, 263, 124357	4.4	3
41	Origin of high hardness and optoelectronic and thermo-physical properties of boron-rich compounds B6X (X = S, Se): A comprehensive study via DFT approach. *Journal of Applied Physics*, **2021**, 129, 175109	2.5	8
40	Physical properties of predicted MAX phase borides Hf2AB (A = Pb, Bi): A DFT insight. *Materials Today Communications*, **2021**, 27, 102411	2.5	3
39	Newly Synthesized Ta-Based MAX Phase (Ta1□Hfx)4AlC3 and (Ta1□Hfx)4Al0.5Sn0.5C3 (0 □x □0.25) Solid Solutions: Unravelling the Mechanical, Electronic, and Thermodynamic Properties. *Physica Status Solidi (B): Basic Research*, **2021**, 258, 2000307	1.3	6
38	Ternary boride Hf3PB4: Insights into the physical properties of the hardest possible boride MAX phase. *Journal of Alloys and Compounds*, **2021**, 857, 158264	5.7	19
37	NaInX2 (X = S, Se) layered materials for energy harvesting applications: first-principles insights into optoelectronic and thermoelectric properties. *Journal of Materials Science: Materials in Electronics*, **2021**, 32, 3878-3893	2.1	4
36	Newly synthesized MAX phase ZrSeC: DFT insights into physical properties towards possible applications.. *RSC Advances*, **2021**, 11, 16892-16905	3.7	9
35	Screen the thermomechanical and optical properties of the new ductile 314 MAX phase boride Zr3CdB4: A DFT insight. *Journal of Alloys and Compounds*, **2021**, 877, 160248	5.7	6
34	Understanding the improvement of thermo-mechanical and optical properties of 212 MAX phase borides Zr2AB2 (A = In, Tl). *Journal of Materials Research and Technology*, **2021**, 15, 2227-2241	5.5	2
33	Effect of sintering temperature on structural and magnetic properties of Ni0.6Zn0.4Fe2O4 ferrite: synthesized from nanocrystalline powders. *Journal of Physics: Conference Series*, **2021**, 1718, 012013	0.3	1

32	Optoelectronic, thermodynamic and vibrational properties of intermetallic MgAl2Ge2: a first-principles study. *SN Applied Sciences*, **2021**, 3, 1	1.8	0
31	Mechanical behavior, enhanced dc resistivity, energy band gap and high temperature magnetic properties of Y-substituted Mg□n ferrites. *Materials Research Express*, **2020**, 7, 036101	1.7	9
30	Dynamical stability, vibrational, and optical properties of anti-perovskite A3BX (Ti3TlN, Ni3SnN, and Co3AlC) phases: A first principles study. *AIP Advances*, **2020**, 10, 095226	1.5	4
29	Recently synthesized (Ti Mo)AlC (0 □□0.20) solid solutions: deciphering the structural, electronic, mechanical and thermodynamic properties simulations.. *RSC Advances*, **2020**, 10, 31535-31546	3.7	22
28	Tailoring the properties of Ni-Zn-Co ferrites by Gd3+ substitution. *Journal of Magnetism and Magnetic Materials*, **2020**, 497, 165978	2.8	18
27	Enhanced dielectric properties of prospective Bi0.85Gd0.15Fe1□r O3 multiferroics. *Results in Physics*, **2019**, 12, 1653-1659	3.7	15
26	Yttrium-substituted Mg□n ferrites: correlation of physical properties with Yttrium content. *Journal of Materials Science: Materials in Electronics*, **2019**, 30, 13258-13270	2.1	9
25	Effects of transition metals on physical properties of M2BC (M = V, Nb, Mo and Ta): A DFT calculation. *Journal of Alloys and Compounds*, **2019**, 770, 523-534	5.7	31
24	Study of physical properties towards optimizing sintering temperature of Y-substituted Mg-Zn ferrites. *Results in Physics*, **2019**, 14, 102517	3.7	14
23	Dielectric and optical properties of Ni-doped LaFeO3 nanoparticles. *SN Applied Sciences*, **2019**, 1, 1	1.8	5
22	First-principles study of elastic, electronic, optical and thermoelectric properties of newly synthesized K2Cu2GeS4 chalcogenide. *Journal of Alloys and Compounds*, **2019**, 781, 37-46	5.7	15
21	Recently synthesized (Zr1-xTix)2AlC (0 □x □1) solid solutions: Theoretical study of the effects of M mixing on physical properties. *Journal of Alloys and Compounds*, **2018**, 743, 146-154	5.7	45
20	Predicted MAX Phase Sc2InC: Dynamical Stability, Vibrational and Optical Properties. *Physica Status Solidi (B): Basic Research*, **2018**, 255, 1700235	1.3	28
19	First principles study of M2InC (M = Zr, Hf and Ta) MAX phases: The effect of M atomic species. *Results in Physics*, **2018**, 11, 869-876	3.7	30
18	Newly synthesized Zr2AlC, Zr2(Al0.58Bi0.42)C, Zr2(Al0.2Sn0.8)C, and Zr2(Al0.3Sb0.7)C MAX phases: A DFT based first-principles study. *Computational Materials Science*, **2017**, 131, 139-145	3.2	43
17	Theoretical investigation of structural, elastic, and electronic properties of ternary boride MoAlB. *Physica Status Solidi (B): Basic Research*, **2017**, 254, 1700010	1.3	79
16	Comparative study of Mo 2 Ga 2 C with superconducting MAX phase Mo 2 GaC: First-principles calculations. *Chinese Physics B*, **2017**, 26, 033102	1.2	24
15	Elastic, thermodynamic and optical behavior of V2AC (A= Al, Ga) MAX phases. *Results in Physics*, **2017**, 7, 3634-3639	3.7	21

14	First-Principles Study of Superconducting ScRhP and ScIrP pnictides. *Physica Status Solidi (B): Basic Research*, **2017**, 254, 1700336	1.3	31
13	First hafnium-based MAX phase in the 312 family, Hf3AlC2: A first-principles study. *Journal of Alloys and Compounds*, **2017**, 727, 616-626	5.7	62
12	Magnetic properties of Sn-substituted Ni□Zn ferrites synthesized from nano-sized powders of NiO, ZnO, Fe 2 O 3 , and SnO 2. *Chinese Physics B*, **2017**, 26, 077501	1.2	6
11	Structural, morphological and electrical properties of Sn-substituted Ni-Zn ferrites synthesized by double sintering technique. *Journal of Magnetism and Magnetic Materials*, **2017**, 424, 148-154	2.8	42
10	First-principles study of SnO under high pressure. *International Journal of Modern Physics B*, **2016**, 30, 1650228	1.1	10
9	New MAX Phase Compound Mo2TiAlC2: First-principles Study. *Journal of Scientific Research*, **2016**, 8, 109-117	1.4	19
8	An ab initio investigation of vibrational, thermodynamic, and optical properties of Sc 2 AlC MAX compound. *Chinese Physics B*, **2016**, 25, 103102	1.2	28
7	Structural, elastic, electronic and optical properties of Cu3MTe4 (M = Nb, Ta) sulvanites □An ab□initio study. *International Journal of Modern Physics B*, **2016**, 30, 1650089	1.1	12
6	First-principles Study of Vickers Hardness and Thermodynamic Properties of Ti3SnC2 Polymorphs. *Journal of Scientific Research*, **2015**, 7, 53-64	1.4	15
5	Structural Properties, Impedance Spectroscopy and Dielectric Spin Relaxation of Ni-Zn Ferrite Synthesized by Double Sintering Technique. *Journal of Scientific Research*, **2015**, 7, 65-75	1.4	28
4	Sulvanite Compounds Cu3TMS4 (TM = V, Nb and Ta): Elastic, Electronic, Optical and Thermal Properties using First-principles Method. *Journal of Scientific Research*, **2014**, 6, 407-419	1.4	24
3	Sn1□BixO2 and Sn1□TaxO2 (0□□0.75): A first-principles study. *Physica B: Condensed Matter*, **2012** , 407, 1020-1026	2.8	14
2	Ni-rich Nitrides ANNi3 (A = Pt, Ag, Pd) in Comparison with Superconducting ZnNNi3. *Journal of Scientific Research*, **2011**, 4, 1	1.4	28
1	Comparative study of predicted MAX phase Hf2AlN with recently synthesized Hf2AlC: a first principle calculations. *Indian Journal of Physics*,1	1.4	2