

## List of Publications by Citations

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

52 papers	765 citations	16 h-index	26 g-index
56 ext. papers	867 ext. citations	2.6 avg, IF	4.13 L-index

#	Paper	IF	Citations
52	First principles prediction of the elastic, electronic, and optical properties of Sb <sub>2</sub> S <sub>3</sub> and Sb <sub>2</sub> Se <sub>3</sub> compounds. <i>Solid State Sciences</i> , <b>2012</b> , 14, 1211-1220	3.4	85
51	The first-principles study on the LaN. <i>Materials Chemistry and Physics</i> , <b>2008</b> , 108, 120-123	4.4	80
50	Structural and mechanical stability of rare-earth diborides. <i>Chinese Physics B</i> , <b>2013</b> , 22, 046202	1.2	53
49	Mechanical, electronic, and optical properties of Bi <sub>2</sub> Se <sub>3</sub> and Bi <sub>2</sub> Te <sub>3</sub> compounds: first principle investigations. <i>Journal of Molecular Modeling</i> , <b>2014</b> , 20, 2180	2	50
48	Mechanical and phonon properties of the superhard LuB <sub>2</sub> , LuB <sub>4</sub> , and LuB <sub>12</sub> compounds. <i>Journal of Alloys and Compounds</i> , <b>2011</b> , 509, 1711-1715	5.7	47
47	The first principles investigation of lattice dynamical and thermodynamical properties of Al <sub>2</sub> Ca and Al <sub>2</sub> Mg compounds in the cubic Laves structure. <i>Computational Materials Science</i> , <b>2013</b> , 68, 27-31	3.2	31
46	The structural and mechanical properties of CdN compound: A first principles study. <i>Computational Materials Science</i> , <b>2011</b> , 50, 3208-3212	3.2	27
45	The first principles studies of the MgB <sub>7</sub> compound: Hard material. <i>Intermetallics</i> , <b>2013</b> , 39, 84-88	3.5	26
44	The effect of hydrogen on the electronic, mechanical and phonon properties of LaMgNi <sub>4</sub> and its hydrides for hydrogen storage applications. <i>International Journal of Hydrogen Energy</i> , <b>2018</b> , 43, 23397-23408	6.7	25
43	Electronic, elastic, thermodynamical, and dynamical properties of the rock-salt compounds LaAs and LaP. <i>Journal of Physics Condensed Matter</i> , <b>2007</b> , 19, 436204	1.8	22
42	The first principles study on boron bismuth compound. <i>Computational Materials Science</i> , <b>2007</b> , 39, 533-540	5.0	22
41	Mechanical and lattice dynamical properties of the Re <sub>2</sub> C compound. <i>Physica Status Solidi - Rapid Research Letters</i> , <b>2010</b> , 4, 347-349	2.5	21
40	Theoretical predictions of the structural, mechanical and lattice dynamical properties of XW <sub>2</sub> (X = Zr, Hf) Laves phases. <i>Philosophical Magazine</i> , <b>2014</b> , 94, 1379-1392	1.6	18
39	Structural and lattice dynamical properties of Zintl NaIn and NaTl compounds. <i>Computational Materials Science</i> , <b>2011</b> , 50, 1070-1076	3.2	18
38	The lattice dynamical and thermo-elastic properties of Rh <sub>3</sub> X (X=Ti, V) compounds. <i>Intermetallics</i> , <b>2010</b> , 18, 286-291	3.5	18
37	Investigation of structural, electronic and anisotropic elastic properties of Ru-doped WB <sub>2</sub> compound by increased valence electron concentration. <i>Materials Chemistry and Physics</i> , <b>2017</b> , 189, 90-95	4.4	16
36	Thermo-elastic and lattice dynamical properties of Rh <sub>3</sub> Hf compound. <i>Computational Materials Science</i> , <b>2010</b> , 48, 859-865	3.2	16

35	Structural, elastic, and lattice dynamical properties of Germanium diiodide (GeI <sub>2</sub> ). <i>Computational Materials Science</i> , <b>2010</b> , 50, 349-355	3.2	15
34	Mechanical and dynamical stability of TiAsTe compound from ab initio calculations. <i>Philosophical Magazine</i> , <b>2015</b> , 95, 2294-2305	1.6	13
33	Stability and morphology-dependence of Sc <sup>3+</sup> ions incorporation and substitution kinetics within ZnO host lattice. <i>Materials Science in Semiconductor Processing</i> , <b>2015</b> , 39, 103-111	4.3	12
32	Density functional study of the mechanical and phonon properties of Al <sub>12</sub> X (X = Mo, Tc, Ru, W, Re, and Os) compounds. <i>Intermetallics</i> , <b>2014</b> , 50, 1-7	3.5	12
31	First-principles studies of the structural, elastic, and lattice dynamical properties of ZrMo <sub>2</sub> and HfMo <sub>2</sub> . <i>Phase Transitions</i> , <b>2017</b> , 90, 598-609	1.3	12
30	Anisotropic elastic and vibrational properties of Ru <sub>2</sub> B <sub>3</sub> and Os <sub>2</sub> B <sub>3</sub> : a first-principles investigation. <i>Materials Research Express</i> , <b>2016</b> , 3, 076501	1.7	12
29	The structural, elastic and vibrational properties of the DyX (X=P, As) compounds. <i>Physica Scripta</i> , <b>2011</b> , 83, 035601	2.6	11
28	Structural, elastic, and lattice dynamical properties of YB <sub>2</sub> compound. <i>Computational Materials Science</i> , <b>2011</b> , 50, 1057-1063	3.2	10
27	Structural, electronic, and elastic properties of K-As compounds: a first principles study. <i>Journal of Molecular Modeling</i> , <b>2012</b> , 18, 3101-12	2	9
26	Molecular structure and vibrational spectra of 4-, 5-, 6-chloroindole. <i>Structural Chemistry</i> , <b>2008</b> , 19, 41-50	1.8	8
25	Scaled DFT Force Constants and Vibrational Spectrum of Cyclopropylamine. <i>Spectroscopy Letters</i> , <b>2005</b> , 38, 505-519	1.1	8
24	Ab initio investigations of the strontium gallium nitride ternaries Sr <sub>3</sub> GaN <sub>3</sub> and Sr <sub>6</sub> GaN <sub>5</sub> : promising materials for optoelectronic. <i>Semiconductor Science and Technology</i> , <b>2013</b> , 28, 085005	1.8	6
23	Vibrational Spectroscopic Studies on the Dicycloheptylaminecobalt(II) Tetracyanonickellate(II) Host-Aromatic Guest Systems. <i>Journal of Inclusion Phenomena and Macrocyclic Chemistry</i> , <b>2005</b> , 53, 219-229		6
22	Synthesis, spectroscopic, crystal structure, biological activities and theoretical studies of 2-[(2E)-2-(2-chloro-6-fluorobenzylidene)hydrazinyl]pyridine. <i>Journal of Molecular Structure</i> , <b>2017</b> , 1135, 98-105	3.4	5
21	Ab-initio calculations on half-Heusler NiXSn (X = Zr, Hf) compounds: electronic and optical properties under pressure. <i>Indian Journal of Physics</i> , <b>2017</b> , 91, 773-778	1.4	5
20	A new quaternary semiconductor compound (Ba <sub>2</sub> Sb <sub>4</sub> GeS <sub>10</sub> ): Ab initio study. <i>Philosophical Magazine</i> , <b>2017</b> , 97, 549-560	1.6	5
19	Electronic structure and related optical, thermoelectric and dynamical properties of Lilianite-type Pb <sub>7</sub> Bi <sub>4</sub> Se <sub>13</sub> : Ab-initio and Boltzmann transport theory. <i>Materialia</i> , <b>2020</b> , 10, 100658	3.2	4
18	First-principles calculations of vibrational and thermodynamical properties of rare-earth diborides. <i>Computational Materials Science</i> , <b>2013</b> , 68, 307-313	3.2	4

17	First principles study on the structural, electronic, and elastic properties of NaAs systems. <i>Solid State Communications</i> , <b>2011</b> , 151, 1349-1354	1.6	4
16	Theoretical study on gas-phase conformations and vibrational assignment of methylphenidate. <i>Computational and Theoretical Chemistry</i> , <b>2009</b> , 893, 17-25		4
15	Calculation of the stability and mechanical and phonon properties of NbRuB, TaRuB, and NbOsB compounds. <i>Philosophical Magazine</i> , <b>2019</b> , 99, 328-346	1.6	4
14	Electronic and thermodynamic properties of lanthanum tetraboride on low-temperature experimental and ab-initio calculation data. <i>Journal of Alloys and Compounds</i> , <b>2021</b> , 862, 158020	5.7	4
13	The stabilities, electronic structures and elastic properties of RbAs systems. <i>Chinese Physics B</i> , <b>2012</b> , 21, 047101	1.2	3
12	Exploring mechanical, electronic, vibrational, and thermoelectric properties of CaGa <sub>2</sub> P <sub>2</sub> , CaGa <sub>2</sub> As <sub>2</sub> , and SrGa <sub>2</sub> As <sub>2</sub> . <i>Solid State Sciences</i> , <b>2019</b> , 96, 105942	3.4	2
11	Conformational and Vibrational Studies of Triclosan <b>2010</b> ,		2
10	Optical and electronic properties of orthorhombic and trigonal AXO <sub>3</sub> (A=Cd, Zn; X=Sn, Ge): First principle calculation. <i>Ferroelectrics</i> , <b>2016</b> , 498, 73-79	0.6	2
9	First-principles investigation of the structural, dynamical, electronic, and elastic properties of WGe <sub>2</sub> and W <sub>5</sub> Ge <sub>3</sub> . <i>Philosophical Magazine</i> , <b>2020</b> , 100, 1129-1149	1.6	1
8	Theoretical investigation of the Anti-Parkinson drug rasagiline and its salts: conformations and infrared spectra. <i>Open Chemistry</i> , <b>2012</b> , 10, 395-406	1.6	1
7	Origin of low thermal conductivity in monolayer PbI <sub>2</sub> . <i>Solid State Communications</i> , <b>2021</b> , 327, 114223	1.6	1
6	2-[(2E)-2-(3-chloro-2-fluorobenzylidene)hydrazinyl]pyridine: Synthesis, spectroscopic, structural properties, biological activity and theoretical analysis. <i>Journal of Molecular Structure</i> , <b>2021</b> , 1227, 129570	3.4	1
5	Strong Elastic Anisotropy of Low-Dimensional Ternary Compounds: InXTe <sub>3</sub> (X = Si, Ge). <i>Journal of Electronic Materials</i> , <b>2021</b> , 50, 2779-2788	1.9	1
4	Revisiting the Electronic Structures and Phonon Properties of Thermoelectric Antimonide-Tellurides: Spin-Orbit Coupling Induced Gap Opening in ZrSbTe and HfSbTe. <i>Crystals</i> , <b>2021</b> , 11, 917	2.3	1
3	Optical and magnetic properties of some XMnSb and Co <sub>2</sub> YZ Compounds: ab initio calculations. <i>Physica Status Solidi C: Current Topics in Solid State Physics</i> , <b>2017</b> , 14, 1600182		1
2	Ab-initio studies of some rare-earth borides: CeB <sub>2</sub> , PrB <sub>2</sub> , NdB <sub>2</sub> , and PmB <sub>2</sub> . <i>International Journal of Materials Research</i> , <b>2013</b> , 104, 858-864	0.5	
1	Stability and Anisotropic Elastic Properties of a Hexagonal BN Compound. <i>Journal of Electronic Materials</i> , <b>1</b>	1.9	