

# Dr Dinesh C GUPTA

## List of Publications by Year in descending order

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180  
papers

3,523  
citations

126907

33  
h-index

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48  
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182  
all docs

182  
docs citations

182  
times ranked

1179  
citing authors

#	ARTICLE	IF	CITATIONS
1	Structural, elastic and thermo-electronic properties of paramagnetic perovskite $\text{PbTaO}_3$ . RSC Advances, 2016, 6, 48009-48015.	3.6	146
2	Robust thermoelectric performance and high spin polarisation in $\text{CoMnTiAl}$ and $\text{FeMnTiAl}$ compounds. RSC Advances, 2016, 6, 80302-80309.	3.6	108
3	Investigation of electronic, magnetic and thermoelectric properties of $\text{Zr}_2\text{NiZ}$ ( $Z = \text{Al, Ga}$ ) ferromagnets. Materials Chemistry and Physics, 2017, 192, 33-40.	4.0	104
4	Investigation of the transport, structural and mechanical properties of half-metallic $\text{REMnO}_3$ ( $\text{RE} = \text{Ce}$ and $\text{Pr}$ ) ferromagnets. RSC Advances, 2016, 6, 97641-97649.	3.6	80
5	Transport, Structural and Mechanical Properties of Quaternary $\text{FeVTiAl}$ Alloy. Journal of Electronic Materials, 2016, 45, 6012-6018.	2.2	70
6	Lattice dynamics, mechanical stability and electronic structure of Fe-based Heusler semiconductors. Scientific Reports, 2019, 9, 1475.	3.3	68
7	Electronic structure, magnetism and thermoelectricity in layered perovskites: $\text{Sr}_2\text{SnMnO}_6$ and $\text{Sr}_2\text{SnFeO}_6$ . Journal of Magnetism and Magnetic Materials, 2017, 441, 166-173.	2.3	65
8	Investigation of electronic structure, magnetic and transport properties of half-metallic $\text{Mn}_2\text{CuSi}$ and $\text{Mn}_2\text{ZnSi}$ Heusler alloys. Journal of Magnetism and Magnetic Materials, 2015, 395, 81-88.	2.3	63
9	Electronic structure, magnetism and thermoelectric properties of double perovskite $\text{Sr}_2\text{HoNbO}_6$ . Journal of Magnetism and Magnetic Materials, 2018, 458, 176-182.	2.3	63
10	Magneto-electronic, thermal, and thermoelectric properties of some Co-based quaternary alloys. Journal of Physics and Chemistry of Solids, 2018, 112, 190-199.	4.0	61
11	Structural, elastic and magneto-electronic properties of half-metallic $\text{BaNpO}_3$ perovskite. Materials Chemistry and Physics, 2017, 198, 380-385.	4.0	60
12	Understanding the origin of half-metallicity and thermophysical properties of ductile $\text{La}_2\text{CuMnO}_6$ double perovskite. International Journal of Energy Research, 2019, 43, 4783-4796.	4.5	59
13	High Pressure-Temperature study on thermodynamics, half-metallicity, transport, elastic and structural properties of Co-based Heusler alloys: A first-principles study. Journal of Solid State Chemistry, 2020, 284, 121178.	2.9	59
14	Thermoelectric and mechanical properties of gapless $\text{Zr}_2\text{MnAl}$ compound. Indian Journal of Physics, 2017, 91, 33-41.	1.8	57
15	Potential lead-free small band gap halide double perovskites $\text{Cs}_2\text{CuMCl}_6$ ( $M = \text{Sb, Bi}$ ) for green technology. Scientific Reports, 2021, 11, 12945.	3.3	51
16	Full-potential study of $\text{Fe}_2\text{NiZ}$ ( $Z = \text{Al, Si, Ga, Ge}$ ). Materials Chemistry and Physics, 2014, 146, 303-312.	4.0	50
17	Effect of on-site Coulomb interaction on electronic and transport properties of 100% spin polarized $\text{CoMnVA}$ s. Journal of Magnetism and Magnetic Materials, 2017, 435, 173-178.	2.3	48
18	Insight into half-metallicity, spin-polarization and mechanical properties of L21 structured $\text{MnY}_2\text{Z}$ ( $Z = \text{Tj, ET, Q, O, Q, r, g, BT, Overlock, 10 T}$ )	5.5	48

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19	Full Heusler alloys (Co <sub>2</sub> TaSi and Co <sub>2</sub> TaGe) as potential spintronic materials with tunable band profiles. <i>Journal of Solid State Chemistry</i> , 2019, 270, 173-179.	2.9	45
20	DFT investigations on mechanical stability, electronic structure and magnetism in Co <sub>2</sub> TaZ (Z = Al, Ga, In) heusler alloys. <i>Semiconductor Science and Technology</i> , 2017, 32, 125019.	2.0	44
21	Magneto-electronic, mechanical, thermoelectric and thermodynamic properties of ductile perovskite Ba <sub>2</sub> SmNbO <sub>6</sub> . <i>Materials Chemistry and Physics</i> , 2020, 239, 121983.	4.0	44
22	New ferromagnetic half-metallic perovskites for spintronic applications: BaMO <sub>3</sub> (M = Mg) Tj ETQq0 0 0 rgBT /Overlock 10 T	3.6	44
23	Analysis of Cage Structured Halide Double Perovskites Cs <sub>2</sub> NaMCl <sub>6</sub> (M = Ti, V) by Spin Polarized Calculations. <i>Journal of Alloys and Compounds</i> , 2021, 854, 156000.	5.5	44
24	Insight into electronic, mechanical and transport properties of quaternary CoVTiAl: Spin-polarized DFT + U approach. <i>Materials Science and Engineering B: Solid-State Materials for Advanced Technology</i> , 2017, 221, 73-79.	3.5	43
25	Investigation of structural, elastic, thermophysical, magneto-electronic, and transport properties of newly tailored Mn-based Heuslers: A density functional theory study. <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26216.	2.0	42
26	Investigation of high pressure and temperature study of thermo-physical properties in semiconducting Fe <sub>2</sub> ZrSi Heusler. <i>Physica B: Condensed Matter</i> , 2020, 577, 411792.	2.7	40
27	Systematic investigation of the magneto-electronic structure and optical properties of new halide double perovskites Cs <sub>2</sub> NaMCl <sub>6</sub> (M = Mn, Co and Ni) by spin polarized calculations. <i>RSC Advances</i> , 2020, 10, 26277-26287.	3.6	40
28	Electronic, mechanical, phase transition and thermo-physical properties of TiC, ZrC and HfC: High pressure computational study. <i>Diamond and Related Materials</i> , 2013, 40, 96-106.	3.9	39
29	Investigation of structural, magneto-electronic, and thermoelectric response of ductile SnAlO <sub>3</sub> from high-throughput DFT calculations. <i>International Journal of Quantum Chemistry</i> , 2017, 117, e25351.	2.0	39
30	Exploration of uranium double perovskites Ba <sub>2</sub> MUO <sub>6</sub> (M = Co, Ni) for magnetism, spintronic and thermoelectric applications. <i>Journal of Magnetism and Magnetic Materials</i> , 2020, 493, 165722.	2.3	39
31	Electronic Structure, Optical and Transport Properties of Double Perovskite La <sub>2</sub> NbMnO <sub>6</sub> : A Theoretical Understanding from DFT Calculations. <i>Journal of Electronic Materials</i> , 2018, 47, 3615-3621.	2.2	38
32	Study of ferromagnetism, spin-polarization, thermoelectrics and thermodynamics of layered perovskite Ba <sub>2</sub> FeMnO <sub>6</sub> under pressure and temperature. <i>Journal of Physics and Chemistry of Solids</i> , 2019, 135, 109079.	4.0	37
33	Scrutinizing the stability and exploring the dependence of thermoelectric properties on band structure of 3d-3d metal-based double perovskites Ba <sub>2</sub> FeNiO <sub>6</sub> and Ba <sub>2</sub> CoNiO <sub>6</sub> . <i>Scientific Reports</i> , 2021, 11, 10506.	3.3	35
34	Investigation of high spin-polarization, magnetic, electronic and half-metallic properties in RuMn <sub>2</sub> Ge and RuMn <sub>2</sub> Sb Heusler alloys. <i>Materials Science and Engineering B: Solid-State Materials for Advanced Technology</i> , 2015, 193, 70-75.	3.5	34
35	Prediction of robustness of electronic, magnetic and thermoelectric properties under pressure and temperature variation in Co <sub>2</sub> MnAs alloy. <i>Computational Condensed Matter</i> , 2019, 19, e00375.	2.1	34
36	Understanding Ferromagnetic Phase Stability, Electronic and Transport Properties of BaPaO <sub>3</sub> and BaNpO <sub>3</sub> from Ab-Initio Calculations. <i>Journal of Electronic Materials</i> , 2017, 46, 5531-5539.	2.2	33

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37	Lanthanum based quaternary Heusler alloys $\text{LaCoCrX}$ ( $X = \text{Al, Ga}$ ): Hunt for half-metallicity and high thermoelectric efficiency. <i>Results in Physics</i> , 2019, 13, 102300.	4.1	33
38	Exploration of electronic structure, mechanical stability, magnetism, and thermophysical properties of $\text{L2}_{1-x}\text{structured Co}_2\text{XSb}$ ( $X = \text{Sc and Ti}$ ) ferromagnets. <i>International Journal of Energy Research</i> , 2020, 44, 2137-2149.	4.5	33
39	Predicting the electronic structure, magnetism, and transport properties of new Co-based Heusler alloys. <i>International Journal of Energy Research</i> , 2018, 42, 4221-4228.	4.5	32
40	Effect of pressure on electronic, magnetic, thermodynamic, and thermoelectric properties of tantalum-based double perovskites $\text{Ba}_2\text{MTaO}_6$ ( $M = \text{Mn, Cr}$ ). <i>International Journal of Energy Research</i> , 2019, 43, 4229-4242.	4.5	32
41	Phase transition and high-pressure elastic behavior of copper halides. <i>Physical Review B</i> , 1989, 40, 11278-11283.	3.2	31
42	A first-principles study of $\text{RuMn}_2\text{Si}$ : Magnetic, electronic and mechanical properties. <i>Journal of Alloys and Compounds</i> , 2013, 575, 292-296.	5.5	30
43	Magnetic, electronic, high-spin polarization and half-metallic properties of $\text{Ru}_2\text{VGe}$ and $\text{Ru}_2\text{VSb}$ Heusler alloys: An FP-LAPW study. <i>Journal of Magnetism and Magnetic Materials</i> , 2015, 374, 209-213.	2.3	30
44	First-principal study of full Heusler alloys $\text{Co}_2\text{VZ}$ ( $Z = \text{As, In}$ ). <i>Journal of Magnetism and Magnetic Materials</i> , 2017, 435, 107-116.	2.3	30
45	Temperature and pressure dependent electronic, mechanical and thermal properties of f-electron based ferromagnetic barium neptunate. <i>Chinese Journal of Physics</i> , 2017, 55, 1769-1779.	3.9	30
46	DFT understandings of structural properties, mechanical stability and thermodynamic properties of $\text{BaCo}_3$ perovskite. <i>Materials Research Express</i> , 2018, 5, 105702.	1.6	30
47	Synthesis and dielectric relaxation studies of Ba substitution in $\text{Pb}(\text{Zn}_{1/3}\text{Nb}_{2/3})\text{O}_3$ ceramics by co-precipitation method. <i>Solid State Sciences</i> , 2010, 12, 1231-1234.	3.2	29
48	Magneto-Electronic, Thermodynamic, and Thermoelectric Properties of 5f-Electron System $\text{BaBkO}_3$ . <i>Journal of Superconductivity and Novel Magnetism</i> , 2019, 32, 1751-1759.	1.8	29
49	A DFT Study on Structural, Electronic Mechanical and Thermodynamic Properties of 5f-Electron System $\text{BaAmO}_3$ . <i>Journal of Superconductivity and Novel Magnetism</i> , 2018, 31, 141-149.	1.8	28
50	First-principles study of high spin-polarization and thermoelectric efficiency of ferromagnetic $\text{CoFeCrAs}$ quaternary Heusler alloy. <i>Journal of Magnetism and Magnetic Materials</i> , 2018, 449, 493-499.	2.3	28
51	Study of the magneto-electronic, optical, thermal and thermoelectric applications of double perovskites $\text{Ba}_2\text{MTaO}_6$ ( $M = \text{Er, Tm}$ ). <i>RSC Advances</i> , 2019, 9, 15852-15867.	3.6	28
52	Pressure-induced phase transitions in silver halides. <i>Physical Review B</i> , 1991, 43, 11185-11189.	3.2	27
53	Structural, electronic, mechanical and thermo-physical properties of TMN ( $\text{TM} = \text{Ti, Zr and Hf}$ ) under high pressures: A first-principle study. <i>International Journal of Refractory Metals and Hard Materials</i> , 2014, 42, 77-90.	3.8	27
54	Electronic, magnetic, elastic and thermodynamic properties of $\text{Cu}_2\text{MnGa}$ . <i>Journal of Magnetism and Magnetic Materials</i> , 2016, 411, 120-127.	2.3	27

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55	Magneto-electronic and thermoelectric properties of some Fe-based Heusler alloys. Journal of Physics and Chemistry of Solids, 2018, 119, 251-257.	4.0	27
56	Electronic structure, mechanical and thermodynamic properties of BaPaO3 under pressure. Journal of Molecular Modeling, 2018, 24, 131.	1.8	26
57	Systematic study of ferromagnetic phase stability of Co-based Heusler materials with high figure of merit: Hunt for spintronics and thermoelectric applicability. AIP Advances, 2020, 10, .	1.3	26
58	A case study of Fe <sub>2</sub> TaZ (Z = Al, Ga, In) Heusler alloys: hunt for half-metallic behavior and thermoelectricity. RSC Advances, 2018, 8, 40996-41002.	3.6	24
59	Quaternary Heusler alloys a future perspective for revolutionizing conventional semiconductor technology. Journal of Alloys and Compounds, 2021, 871, 159560.	5.5	24
60	Thermoelectric response of ZrNiSn and ZrNiPb Half-Heuslers: Applicability of semi-classical Boltzmann transport theory. Results in Physics, 2019, 12, 1382-1386.	4.1	23
61	Structural, elastic, thermodynamic and thermoelectric properties of Fe <sub>2</sub> TiSn Heusler alloy: High pressure study. Results in Physics, 2019, 12, 15-20.	4.1	23
62	Exploration of highly correlated Co-based quaternary Heusler alloys for spintronics and thermoelectric applications. International Journal of Energy Research, 2019, 43, 8864.	4.5	22
63	Magneto-electronic, thermoelectric, thermodynamic and optical properties of rare earth YCoTiX (X=) Tj ETQq1 1 0,784314 rgBT /Ove	5.5	21
64	High-Temperature and High-Pressure Study of Electronic and Thermal Properties of PbTaO3 and SnAlO3 Metal Perovskites by Density Functional Theory Calculations. Journal of Electronic Materials, 2018, 47, 436-442.	2.2	20
65	Ternary germanide Li <sub>2</sub> ZnGe: A new candidate for high temperature thermoelectrics. Journal of Alloys and Compounds, 2018, 738, 501-508.	5.5	19
66	Silicon Epitaxial Layers with Abrupt Interface Impurity Profiles. Journal of the Electrochemical Society, 1969, 116, 1561.	2.9	18
67	Insight into mechanical properties and thermoelectric efficiency of Zr <sub>2</sub> CoZ (Z=Si, Ge) Heusler alloys. Materials Research Express, 2017, 4, 116307.	1.6	18
68	Analysis of electronic, thermal, and thermoelectric properties of the half-Heusler CrTiSi material using density functional theory. Journal of Physics and Chemistry of Solids, 2018, 119, 281-287.	4.0	18
69	Phase stability, ductility, electronic, elastic and thermo-physical properties of TMNs (TM=V, Nb and Ta): An ab initio high pressure study. Computational Materials Science, 2014, 90, 182-195.	3.0	17
70	Temperature and pressure dependent structural and thermo-physical properties of quaternary CoVTiAl alloy. Journal of Physics and Chemistry of Solids, 2017, 108, 109-114.	4.0	17
71	Unravelling the magnetism, high spin polarization and thermoelectric efficiency of ZrFeSi half-Heusler. Physica B: Condensed Matter, 2018, 534, 5-9.	2.7	17
72	First principle study of mechanical stability, magneto-electronic and thermodynamic properties of double perovskites: A <sub>2</sub> MgWO <sub>6</sub> (A=Ca, Sr). Materials Science and Engineering B: Solid-State Materials for Advanced Technology, 2019, 250, 114434.	3.5	16

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73	Electronic, ductile, phase transition and mechanical properties of Lu-monopnictides under high pressures. <i>Journal of Molecular Modeling</i> , 2013, 19, 5343-5354.	1.8	15
74	<math>\delta</math>-band gap halide double perovskite for optoelectronic properties. <i>International Journal of Energy Research</i> , 2021, 45, 7222-7234.	4.5	15
75	Structural and mechanical stabilities, electronic, magnetic and thermophysical properties of double perovskite $\text{Ba}_2\text{LaNb}_6\text{O}_{26}$ : Probed by DFT computation. <i>International Journal of Energy Research</i> , 2021, 45, 14603-14611.	4.5	15
76	Poly-schiff bases II. Synthesis and characterization of polyetherketoimines. <i>European Polymer Journal</i> , 1996, 32, 661-664.	5.4	14
77	Pressure induced magnetic, electronic and mechanical properties of $\text{SmX}$ (X = Se, Te). <i>Journal of Physics Condensed Matter</i> , 2009, 21, 436011.	1.8	14
78	Insight view of double perovskites $\text{Ba}_2\text{XNb}_6\text{O}_{26}$ ( $\text{X}=\text{Ho, Yb}$ ) for spintronics and thermoelectric applications. <i>International Journal of Energy Research</i> , 2021, 45, 13338-13354.	4.5	14
79	Pursuit of thermoelectric properties in L21 structured $\text{Co}_2\text{PAI}$ (P = Ru, Rh) ductile ferromagnetic materials: A first principles prospective. <i>Journal of Solid State Chemistry</i> , 2021, 296, 121942.	2.9	13
80	New isostructural halide double perovskites $\text{Cs}_2\text{GeNiX}_6$ (X= Cl, Br) for semiconductor spintronics and thermoelectric advancements. <i>Journal of Solid State Chemistry</i> , 2021, 300, 122196.	2.9	13
81	Structural phase transition, elastic and electronic properties of $\text{TmSb}$ and $\text{YbSb}$ : A LSDA + U study under pressure. <i>Journal of Alloys and Compounds</i> , 2012, 515, 26-31.	5.5	12
82	Chemical Potential Evaluation of Thermoelectric and Mechanical Properties of $\text{Zr}_2\text{CoZ}$ (Z=Si, Ge) Heusler Alloys. <i>Journal of Electronic Materials</i> , 2018, 47, 2468-2478.	2.2	12
83	Current research and future prospective of cobalt-based Heusler alloys as thermoelectric materials: A density functional approach. <i>International Journal of Energy Research</i> , 2021, 45, 4652-4668.	4.5	12
84	High temperature and pressure dependent structural and thermophysical properties of $\text{Co}_2\text{VN}$ (N = Sn, Sb) ferromagnetic materials. <i>Materials Research Express</i> , 2020, 7, 125701.	1.6	12
85	Synthesis and characterisation of some new cyanonitrosyl chromium(II) complexes with phenetidines and anisidines. <i>Transition Metal Chemistry</i> , 1986, 11, 463-464.	1.4	11
86	Effect of high pressure on polymorphic phase transition and electronic structure of XAs (X=Al, Ga). <i>Tj ETQq0 0 0 rgBTj/Overlock 10 Tf 50</i>	1.3	11
87	Impedance spectroscopy of perovskite barium substituted lead zinc niobate ceramics. <i>Physica B: Condensed Matter</i> , 2010, 405, 1608-1614.	2.7	11
88	Effect of covalency, zero-point energy and charge transfer on the phase-transition, elastic and thermophysical properties of Ca-chalcogenides under compression. <i>Phase Transitions</i> , 2010, 83, 182-194.	1.3	11
89	Sunspots and geomagnetic storms during solar cycle-23. <i>Indian Journal of Physics</i> , 2012, 86, 563-567.	1.8	11
90	Effect of solar wind plasma parameters on space weather. <i>Research in Astronomy and Astrophysics</i> , 2015, 15, 85-106.	1.7	11

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91	Pressure- and Temperature-Dependent Study of Heusler Alloys Cu <sub>2</sub> MGa (M = Cr and V). Journal of Electronic Materials, 2017, 46, 2185-2195.	2.2	11
92	Effect of 3d transition metal doping (Co, Ni and Cu) on structural, optical, morphological and dielectric properties of sol-gel assisted auto-combusted Mg <sub>0.95</sub> Mn <sub>0.05</sub> O nanoparticles. Journal of Materials Science: Materials in Electronics, 2018, 29, 3952-3956.	2.2	11
93	Electronic and Transport Properties of LaNi <sub>4</sub> Sb <sub>12</sub> Skutterudite: Modified Becke-Johnson Approach. Journal of Electronic Materials, 2018, 47, 4544-4549.	2.2	11
94	Investigation of structural and mechanical properties of ferromagnetic Co <sub>2</sub> MnAs compound. AIP Conference Proceedings, 2019, . .	0.4	11
95	Structural, Magneto-electronic, Mechanical, and Thermophysical Properties of Double Perovskite Ba <sub>2</sub> ZnReO <sub>6</sub> . Physica Status Solidi (B): Basic Research, 2019, 256, 1800625.	1.5	11
96	Investigation of Electronic, Magnetic, Thermodynamic, and Thermoelectric Properties of Half-Metallic XLiSn (X = Ce, Nd) Alloys. Journal of Superconductivity and Novel Magnetism, 2019, 32, 2009-2019.	1.8	11
97	Comprehensive DFT investigation of transition-metal-based new quaternary Heusler alloys CoNbMnZ (Z = Ge, Sn): compatible for spin-dependent and thermoelectric applications. RSC Advances, 2020, 10, 43870-43881.	3.6	11
98	Intrinsic magnetism and thermoelectric applicability of novel halide perovskites Cs <sub>2</sub> GeMnX <sub>6</sub> (X = Cl, I). Engineering B: Solid-State Materials for Advanced Technology, 2021, 265, 114985.	3.5	11
99	Study of the anharmonic properties of copper halides. Nuovo Cimento Della Societa Italiana Di Fisica D - Condensed Matter, Atomic, Molecular and Chemical Physics, Biophysics, 1987, 9, 1253-1264.	0.4	10
100	Analysis of mechanical, thermodynamic, and thermoelectric properties of ferromagnetic SrFe <sub>4</sub> As <sub>12</sub> skutterudite. Journal of Solid State Chemistry, 2018, 266, 274-278.	2.9	10
101	Electronic, elastic and thermoelectric performance in n-type Sr-filled brittle skutterudite. Physica B: Condensed Matter, 2020, 592, 412209.	2.7	10
102	Effect of variation of metal and non-metal elements on various properties of rare-earth-based inverse perovskites Gd <sub>3</sub> XY (X = Ga, In and Y = B, N). International Journal of Quantum Chemistry, 2020, 120, e26197.	2.0	10
103	Understanding the origin of semiconducting ferromagnetic character along with the high figure of merit in Cs <sub>2</sub> NaMCl <sub>6</sub> (M = Cr, Fe) double perovskites. Journal of Magnetism and Magnetic Materials, 2021, 519, 167431.	2.3	10
104	Robustness in ferromagnetic phase stability, half-metallic behavior and transport properties of cobalt-based Heuslers compounds: A first principles approach. International Journal of Quantum Chemistry, 2021, 121, e26538.	2.0	10
105	Non-destructive determination of carrier concentration in epitaxial silicon using a total internal reflection technique. Solid-State Electronics, 1970, 13, 543-552.	1.4	9
106	Pressure-induced phase transitions and electronic structure of GaAs. Journal of Physics Condensed Matter, 2008, 20, 255204.	1.8	9
107	Structural and elastic properties of copper iodide. Physica B: Condensed Matter, 2010, 405, 133-139.	2.7	9
108	High pressure phase-transition, elastic and thermal properties of uranium chalcogenides: A model study. Journal of Alloys and Compounds, 2010, 499, 90-97.	5.5	9

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109	Thermal, electronic and ductile properties of lead-chalcogenides under pressure. Journal of Molecular Modeling, 2013, 19, 3481-3489.	1.8	9
110	Effect of High Pressure and Temperature on Structural, Thermodynamic and Thermoelectric Properties of Quaternary CoFeCrAl Alloy. Journal of Electronic Materials, 2018, 47, 2042-2049.	2.2	9
111	Investigation of spin polarized band structure, magnetism, and mechanical properties of new gapless Zr <sub>2</sub> NbX (X= Al, Ga, In) Heusler alloys. Journal of Alloys and Compounds, 2018, 766, 241-247.	5.5	9
112	Analysing cation-modified magnetic perovskites A <sub>2</sub> SnFeO <sub>6</sub> (A = Ca, Ba): a DFT study. RSC Advances, 2021, 11, 27499-27511.	3.6	9
113	Direct Measurement of Impurity Distribution in Semiconducting Materials. Journal of Applied Physics, 1972, 43, 515-522.	2.5	8
114	High pressure phase transitions and elastic properties of IV-VI compound semiconductors. Phase Transitions, 1995, 53, 39-51.	1.3	8
115	Analysis of magneto-electronic, thermodynamic and thermoelectric properties of ferromagnetic CoFeCrAl alloy. Materials Research Express, 2017, 4, 116103.	1.6	8
116	Insight into various properties of rare-earth based inverse perovskites Gd <sub>3</sub> AlX (X = B, N). International Journal of Energy Research, 2020, 44, 1654-1672.	4.5	8
117	Determination of Mobility and Its Profile in n/n+ Silicon Epitaxial Layers. Journal of the Electrochemical Society, 1969, 116, 670.	2.9	7
118	Anharmonic Properties of IV-VI Compound Semiconductors. Physica Status Solidi (B): Basic Research, 1988, 149, 121-125.	1.5	7
119	High-pressure phase transitions in Cu <sub>x</sub> Ag <sub>1-x</sub> mixed crystals. Physical Review B, 1992, 45, 7031-7035.	3.2	7
120	Magnetic, Electronic, and Mechanical Properties of Strongly Correlated Samarium Mono-chalcogenides under High Pressure. Journal of the Physical Society of Japan, 2010, 79, 044605.	1.6	7
121	DySb under high pressures: A full-potential study. Journal of Alloys and Compounds, 2011, 509, 4653-4659.	5.5	7
122	Effect of High Pressure and Temperature on Magneto-Electronic, Thermodynamic, and Transport Properties of Antiferromagnetic HoPdX (X=As, Ge) Alloys. Journal of Superconductivity and Novel Magnetism, 2019, 32, 2051-2065.	1.8	7
123	Systematic understanding of f-electron based semiconducting actinide perovskites Ba <sub>2</sub> MgMO <sub>6</sub> (M = U, Np) from DFT ab initio calculations. International Journal of Energy Research, 2020, 44, 3066-3081.	4.5	7
124	Electronic, mechanical, phase transition, and thermo-physical properties of TMC (TM = V, Nb, and Ta): high pressure ab initio study. Phase Transitions, 2015, 88, 1193-1212.	1.3	6
125	High-Pressure and Temperature Dependence of Electronic, Magnetic, Elastic, Thermodynamic, and Transport Properties of Full-Heusler Alloys Co <sub>2</sub> YIn (Y = Nb, Zr). Journal of Superconductivity and Novel Magnetism, 2018, 31, 2465-2483.	1.8	6
126	DFT investigations on the electronic structure, magnetism, thermodynamic and elastic properties of newly predicted cobalt based antiperovskites: Co <sub>3</sub> XN (X=Pt, Rh). Results in Physics, 2020, 17, 103112.	4.1	6



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127	High temperature and pressure study on structural and thermophysical properties of $\text{Co}_2\text{XAl}$ (X = Zr, Nb, Hf) Heusler materials by density functional theory calculations. Philosophical Magazine, 2021, 101, 1654-1678.	1.6	6
128	Structural properties of silver iodide and copper iodide. Open Physics, 2008, 6, .	1.7	5
129	Thermal and elastic properties of thorium pnictides under high pressure. Phase Transitions, 2010, 83, 404-418.	1.3	5
130	Study of semiconducting nanomaterials under pressure. Journal of Molecular Modeling, 2012, 18, 3341-3350.	1.8	5
131	Half-metallicity and onsite Hubbard interaction on d-electronic states: a case study of $\text{Fe}_2\text{NiZ}$ (Z = Al, Tj) $\text{E}_{\text{Q1}} = 1.0784314$ eV	1.6	5
132	Evaluation of mechanical and transport properties of $\text{Zr}_2\text{CoSi}$ Heusler alloy. AIP Conference Proceedings, 2017, , .	0.4	4
133	Robustness in spin polarization and thermoelectricity in newly tailored Mn <sup>2+</sup> -based Heusler alloys. Indian Journal of Physics, 2018, 92, 855-864.	1.8	4
134	Electronic structure, mechanical, thermoelectric, optical, and thermodynamic properties of yttrium-based quaternary Heusler alloys. International Journal of Energy Research, 2019, 43, 8633.	4.5	4
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