

# G Kalpana

## List of Publications by Year in descending order

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58  
papers

939  
citations

567281

15  
h-index

454955

30  
g-index

59  
all docs

59  
docs citations

59  
times ranked

712  
citing authors

#	ARTICLE	IF	CITATIONS
1	Electronic structure and structural phase stability in BaS, BaSe, and BaTe. Physical Review B, 1994, 50, 12318-12325.	3.2	106
2	Electronic and structural properties of alkaline-earth oxides under high pressure. Physical Review B, 1995, 52, 4-7.	3.2	81
3	Electronic and structural properties of MgS and MgSe. Physica B: Condensed Matter, 1996, 222, 223-228.	2.7	76
4	First-principles study of electronic structure and ground-state properties of alkali-metal sulfides $\text{Li}_2\text{S}$ , $\text{Na}_2\text{S}$ , $\text{K}_2\text{S}$ and $\text{Rb}_2\text{S}$ . Physica Status Solidi (B): Basic Research, 2007, 244, 1337-1346.	1.5	59
5	Ab-initio investigation of half-metallic ferromagnetism in half-Heusler compounds XYZ (X=Li, Na, K and) Tj ETQq1 1 0,784314,rgBT /Over	2.3	59
6	Structural and Electronic Properties of SrS, SrSe, and SrTe Under Pressure. Journal of Low Temperature Physics, 1998, 112, 211-226.	1.4	57
7	Ab initio Electronic Band Structure Calculations for Beryllium Chalcogenides. International Journal of Modern Physics B, 1998, 12, 1975-1984.	2.0	55
8	Structural and electronic properties of alkaline-earth fluorohalides under pressure. Physical Review B, 1997, 56, 3532-3535.	3.2	45
9	Ab Initio Electronic Band Structure Calculations for Calcium Monochalcogenides. International Journal of Modern Physics B, 1998, 12, 1709-1717.	2.0	39
10	Reduced graphene oxide/strontium titanate heterostructured nanocomposite as sunlight driven photocatalyst for degradation of organic dye pollutants. Current Applied Physics, 2018, 18, 1026-1033.	2.4	36
11	Electronic structure and ground-state properties of alkali-metal oxides $\text{Li}_2\text{O}$ , $\text{Na}_2\text{O}$ , $\text{K}_2\text{O}$ and $\text{Rb}_2\text{O}$ : A first-principles study. Physica B: Condensed Matter, 2007, 396, 124-131.	2.7	29
12	Theoretical study of electronic, magnetic and structural properties of Mo and W based group V (N, P,) Tj ETQq0 0 0,rgBT /Overlock 10 T	3.8	26
13	FIRST-PRINCIPLES STUDY OF ELECTRONIC STRUCTURE AND GROUND-STATE PROPERTIES OF ALKALI-METAL SELENIDES AND TELLURIDES $(M_{2}A)$ [M: Li, Na, K; A: Se, Te]. International Journal of Modern Physics B, 2009, 23, 5027-5037.	2.0	24
14	First-Principles Calculation of structural, electronic and magnetic properties of half-Heusler LiCaC and NaCaC compounds. Physica B: Condensed Matter, 2014, 448, 256-259.	2.7	24
15	Electronic and structural properties of $\text{NaZnX}$ (X = P, As, Sb): an ab initio study. Journal of Physics Condensed Matter, 2008, 20, 085220.	1.8	23
16	Half-metallic ferromagnetism in alkaline earth selenides by first principles calculations. Computational Materials Science, 2012, 54, 219-226.	3.0	15
17	Electronic Structure and Superconductivity of NbN under High Pressure. Physica Status Solidi (B): Basic Research, 1993, 176, 195-202.	1.5	13
18	Influence of $\text{RGO/TiO}_2$ nanocomposite on photo-degrading Rhodamine B and Rose Bengal dye pollutants. Bulletin of Materials Science, 2018, 41, 1.	1.7	12

#	ARTICLE	IF	CITATIONS
19	Prediction of structural, electronic and magnetic properties of full Heusler alloys Ir <sub>2</sub> YSi (Y = Sc, Ti, V). <i>Tj ETQq1 1 0.784314 rgBT /Overlock 10</i>	1.3	12
20	Superconductivity of WC in the NaCl-Type Structure under Pressure. <i>Japanese Journal of Applied Physics</i> , 1994, 33, 1847-1850.	1.5	11
21	Electronic properties and structural phase transition in A <sub>4</sub> [M <sub>4</sub> O <sub>4</sub> ] (A=Li, Na, K and Rb; M=Ag and Cu): A first principles study. <i>Solid State Communications</i> , 2013, 155, 62-68.	1.9	11
22	Pressure induced structural phase transition in SnS " An ab initio study. <i>Bulletin of Materials Science</i> , 2006, 29, 25-28.	1.7	10
23	Band structure and superconductivity of BCC tellurium under pressure. <i>Physica B: Condensed Matter</i> , 1993, 191, 287-292.	2.7	9
24	First-principles study of structural, electronic and magnetic properties of AeX (Ae=Be, Mg, Sr, Ba; X=Si). <i>Tj ETQq0 0,0 rgBT /Overlock 10</i>	2.3	9
25	Electronic structure and magnetic properties of chalcopyrite type ZnMX <sub>2</sub> (M=Sc, V, Cr, Mn, Fe; X=P, As), compounds: An ab initio study. <i>Physica Status Solidi (B): Basic Research</i> , 2016, 253, 1576-1584.	1.5	9
26	DFT studies on electronic, magnetic and thermoelectric properties of half Heusler alloys XCaB (X=Li). <i>Tj ETQq0 0,0 rgBT /Overlock 10</i>	1.5	9
27	Electronic structure and half-metallic ferromagnetism in (C, Si, Ge and Sn) doped alkaline-earth sulfides: A first principles approach. <i>Journal of Alloys and Compounds</i> , 2013, 573, 83-89.	5.5	8
28	Pressure induced magnetic phase transition in Fe <sub>3</sub> Pt. <i>Journal of Alloys and Compounds</i> , 1996, 240, 124-127.	5.5	7
29	Half-metallic ferromagnetism in (C, Si, Ge, Sn and Pb)-doped I <sub>2</sub> VI compounds: An ab initio study. <i>Journal of Physics and Chemistry of Solids</i> , 2011, 72, 227-232.	4.0	7
30	Physical Properties of Thorium under Pressure. <i>Physica Status Solidi (B): Basic Research</i> , 1993, 178, 185-197.	1.5	5
31	Structural Phase Stability in BaSe. <i>Physica Status Solidi (B): Basic Research</i> , 1994, 184, 153-157.	1.5	5
32	Structural phase stability of ThSb and ThAs under pressure. <i>Bulletin of Materials Science</i> , 1997, 20, 597-600.	1.7	5
33	Half-metallic ferromagnetism in I <sub>2</sub> VI compounds with non-magnetic dopants. <i>Solid State Communications</i> , 2011, 151, 1169-1174.	1.9	5
34	First principles study of half-metallic ferromagnetism in (N, P, As and Sb) doped alkaline-earth sulfides. <i>Computational Materials Science</i> , 2012, 65, 426-433.	3.0	5
35	Half-metallic ferromagnetism in full-Heusler compounds ACaX <sub>2</sub> (A = K and Rb; X = N and O)., 2014, , .		5
36	Investigation of novel quaternary Heusler alloys XRuCrZ (X = Co, Ni, Rh, and Pd; Z = Si and Ge) via first-principles calculation for spintronics and thermoelectric applications. <i>AIP Advances</i> , 2022, 12, .	1.3	5

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37	A structural study on MFCl (M=Ca, Sr, Ba) and BaFX (X=Br, I). Bulletin of Materials Science, 1997, 20, 461-465.	1.7	3
38	Ab initio electronic band structure calculations of half-metallic calcium pnictides. Physica Status Solidi (B): Basic Research, 2007, 244, 4643-4650.	1.5	3
39	Half metallic ferromagnetism in ACaB (A = Li, Na and K) compounds-DFT study. , 2013, , .		3
40	Investigation of graphene based NiS nanocomposite by solvothermal method for energy storage application. Materials Letters: X, 2021, 12, 100112.	0.7	3
41	Band structure and superconductivity of ZrN under high pressure. Journal of Alloys and Compounds, 1993, 202, 51-56.	5.5	2
42	Magnetism induced by nonmagnetic dopant in Li <sub>2</sub> O, Na <sub>2</sub> O, K <sub>2</sub> O and Rb <sub>2</sub> O: first-principles calculations. Journal of Materials Science, 2012, 47, 2316-2321.	3.7	2
43	First principle calculations on structural, electronic, and magnetic properties of CdMAs <sub>2</sub> (M = Sc, Ti,) Tj ETQq1 1 0.784314 rgBT /Overlock	1.1	2
44	Structural Phase Stability of ThSb Under Pressure. Materials Research Society Symposia Proceedings, 1994, 364, 1095.	0.1	1
45	Half-Metallic Ferromagnetism In Calcium Chalcogenides In The Presence Of Nonmagnetic Impurities (B,) Tj ETQq1 1 0.784314 rgBT /C	0.4	1
46	Electronic and Magnetic Properties of CaS <sub>0.875</sub> M <sub>0.125</sub> (M = C, Si, Ge and Sn) by First Principles Theory. Journal of Physics: Conference Series, 2012, 377, 012073.	0.4	1
47	Half-Metallic Ferromagnetism in MgS by Doping with &lt;i>Sp</i>-Element: A First-Principles Calculations. Advanced Materials Research, 0, 665, 22-28.	0.3	1
48	Electronic and magnetic properties of CdI <sub>2</sub> -type MX <sub>2</sub> (M = V, Nb; X = Al, Ga and) Tj ETQq0 0 0 rgBT /Overlock	0.6	1
49	Band structure and superconductivity of bcc tellurium under pressure. AIP Conference Proceedings, 1994, , .	0.4	0
50	Electronic structure and physical properties of bcc selenium under high pressure. High Pressure Research, 1994, 12, 111-118.	1.2	0
51	Magnetism induced by sp dopant in Ionic Insulator (Li <sub>2</sub> O): A DFT Study. , 2011, , .		0
52	2p Elements Induced Half-Metallic Ferromagnetism in Alkaline Earth Chalcogenides. , 2011, , .		0
53	Electronic structure and ground state properties of A <sub>4</sub> [Cu <sub>4</sub> O <sub>4</sub> ] (A=Li, Na, K and Rb): A first principle study. , 2012, , .		0
54	Half-metallic ferromagnetism in MgS <sub>0.875</sub> X <sub>0.125</sub> (X = C, Si, Ge and Sn): A first principle approach. , 2012, , .		0

#	ARTICLE	IF	CITATIONS
55	Electronic and magnetic properties of ASrB (A=Li, Na, K and Rb) compounds: First principles study. , 2013, , .		0
56	Electronic Structure and Ground State Properties of A<sub>4</sub>[Ag<sub>4</sub>O<sub>4</sub>] (A=Na, K and Rb): A First-Principles Study. Advanced Materials Research, 0, 665, 43-48.	0.3	0
57	Half-metallic ferromagnetism in chalcopyrite type compounds ZnMX <sub>2</sub> (M=Sc, V, Mn, Fe; X = P, As). AIP Conference Proceedings, 2015, , .	0.4	0
58	A Facile Synthesis of PbS-G QDs Nanocomposite as Electrode Material with Enhanced Energy Density for High Performance Supercapattery Application. Journal of Inorganic and Organometallic Polymers and Materials, 2022, 32, 2135-2145.	3.7	0