Dibya Prakash Rai

List of Publications by Citations

204 papers	1,847 citations	21 h-index	31 g-index
223 ext. papers	2,479 ext. citations	2.7 avg, IF	5.36 L-index

#	Paper	IF	Citations
204	Structural, electronic and magnetic properties of Fe2-based full Heusler alloys: A first principle study. *Journal of Magnetism and Magnetic Materials*, **2016**, 407, 167-174	2.8	55
203	First-principles computations of (hbox {Y}_{x}hbox {Ga}_{1-{x}})As-ternary alloys: a study on structural, electronic, optical and elastic properties. *Bulletin of Materials Science*, **2020**, 43, 1	1.7	53
202	Electronic, optical and thermoelectric investigations of Zintl phase AE3AlAs3 (AE = Sr, Ba): First-principles calculations. *Chinese Journal of Physics*, **2018**, 56, 870-879	3.5	51
201	High-pressure synthesis, crystal structures, and magnetic properties of 5d double-perovskite oxides Ca2MgOsO6 and Sr2MgOsO6. *Inorganic Chemistry*, **2015**, 54, 3422-31	5.1	48
200	Theoretical prediction of electronic, transport, optical, and thermoelectric properties of Janus monolayers In2XO (X=S,Se,Te). *Physical Review B*, **2021**, 103,	3.3	39
199	A new multi-objective Jaya algorithm for optimization of modern machining processes. *Advances in Production Engineering and Management*, **2016**, 11, 271-286	2.5	38
198	Ba2NiOsO6: A Dirac-Mott insulator with ferromagnetism near 100 K. *Physical Review B*, **2016**, 94,	3.3	36
197	Study of Co2MnAl Heusler alloy as half metallic ferromagnet. *Indian Journal of Physics*, **2010**, 84, 717-721	1.4	35
196	The electronic, magnetic and optical properties of double perovskite A2FeReO6 (A = Sr, Ba) from first principles approach. *Computational Materials Science*, **2015**, 101, 313-320	3.2	34
195	Study of the enhanced electronic and thermoelectric (TE) properties of ZrxHf1□□TayNiSn: a first principles study. *RSC Advances*, **2015**, 5, 95353-95359	3.7	34
194	A comparative study of a Heusler alloy Co2FeGe using LSDA and LSDA+U. *Physica B: Condensed Matter*, **2012**, 407, 3689-3693	2.8	33
193	A promising thermoelectric response of HfRhSb half Heusler compound at high temperature: A first principle study. *Journal of Alloys and Compounds*, **2018**, 763, 1018-1023	5.7	31
192	Electronic and optical properties of cubic SrHfO3 at different pressures: A first principles study. *Materials Chemistry and Physics*, **2017**, 186, 620-626	4.4	31
191	A tunneling current density model for ultra thin HfO2 high-k dielectric material based MOS devices. *Superlattices and Microstructures*, **2016**, 95, 24-32	2.8	29
190	Doping-Induced Half-Metallic Ferromagnetism in Vanadium and Chromium-Doped Alkali Oxides K2O and Rb2O: Ab Initio Method. *Journal of Superconductivity and Novel Magnetism*, **2017**, 30, 2197-2210	1.5	28
189	A DFT study of BeX (X = S, Se, Te) semiconductor: Modified Becke Johnson (mBJ) potential. *Semiconductors*, **2014**, 48, 1411-1422	0.7	27
188	Electronic structure and elastic properties of scandium carbide and yttrium carbide: A first principles study. *Physica B: Condensed Matter*, **2011**, 406, 4041-4045	2.8	27

187	Study of energy bands and magnetic properties of Co2CrSi Heusler alloy. *Bulletin of Materials Science*, **2011**, 34, 1219-1222	1.7	26
186	Electronic, elastic and X-ray spectroscopic properties of direct and inverse full Heusler compounds Co2FeAl and Fe2CoAl, promising materials for spintronic applications: a DFT+U approach. *Journal of Materials Chemistry C*, **2018**, 6, 10341-10349	7.1	23
185	Electronic, optical, and thermoelectric properties of Fe2+xV1−xAl. *AIP Advances*, **2017**, 7, 045118	1.5	22
184	Possible half-metallic antiferromagnetism in an iridium double-perovskite material. *Physical Review B*, **2016**, 93,	3.3	22
183	Effect of point defects on the electronic density states of SnC nanosheets: First-principles calculations. *Results in Physics*, **2017**, 7, 3209-3215	3.7	21
182	Study of electronic and magnetic properties in 4felectron based cubic EuAlO3: a first-principles calculation. *Physica Scripta*, **2015**, 90, 065803	2.6	21
181	Electronic and magnetic properties of X2YZ and XYZ Heusler compounds: a comparative study of density functional theory with different exchange-correlation potentials. *Materials Research Express*, **2016**, 3, 075022	1.7	21
180	Mechanical stability and thermoelectric properties of the PdZrTiAl quaternary Heusler: A DFT study. *Solid State Communications*, **2020**, 308, 113838	1.6	19
179	Optical and electronic properties of pure and fully hydrogenated SiC and GeC nanosheets: first-principles study. *Optical and Quantum Electronics*, **2018**, 50, 1	2.4	19
178	Prediction of half-metallic ferromagnetism (HMF) in hypothetical Heusler compound Co2VSb using modified Becke Johnson (mBJ) potential. *Journal of Alloys and Compounds*, **2014**, 589, 553-557	5.7	19
177	An abinitio study of the half-metallic properties of Co2TGe (T=Sc, Ti, V, Cr, Mn, Fe): LSDA+U method. *Journal of the Korean Physical Society*, **2013**, 62, 1652-1660	0.6	19
176	Structural, electronic, mechanical, and thermoelectric properties of a novel half Heusler compound HfPtPb. *Journal of Applied Physics*, **2017**, 122, 045110	2.5	19
175	Study of DOS and energy band structures in beryllium chalcogenides. *Indian Journal of Physics*, **2011** , 85, 727-736	1.4	19
174	Spin-induced transition metal (TM) doped SnO2 a dilute magnetic semiconductor (DMS): A first principles study. *Journal of Physics and Chemistry of Solids*, **2018**, 120, 104-108	3.9	18
173	Study of electronic, magnetic, optical and elastic properties of Cu2MnAl a gapless full Heusler compound. *Journal of Alloys and Compounds*, **2014**, 612, 355-360	5.7	18
172	Study of Interface Charge Densities for ZrO2and HfO2Based Metal-Oxide-Semiconductor Devices. *Advances in Materials Science and Engineering*, **2014**, 2014, 1-6	1.5	18
171	Creating Weyl nodes and controlling their energy by magnetization rotation. *Physical Review Research*, **2019**, 1,	3.9	18
170	Image Force Effect on Tunneling Current for Ultra Thin High-K Dielectric Material Al2O3 Based Metal Oxide Semiconductor Devices. *Journal of Nanoelectronics and Optoelectronics*, **2015**, 10, 645-648	1.3	18

169	Study of 5f electron based filled skutterudite compound EuFe4Sb12, a thermoelectric (TE) material: FP-LAPW method. *Journal of Alloys and Compounds*, **2015**, 619, 621-626	5.7	17
168	Controlling the electronic and optical properties of HfS mono-layers lanthanide substitutional doping: a DFT+ study.. *RSC Advances*, **2020**, 10, 15670-15676	3.7	16
167	Ground state properties of filled skutterudite EuRu4P12: A first principles study. *Journal of Alloys and Compounds*, **2013**, 578, 559-564	5.7	16
166	ELECTRONIC STRUCTURE AND MAGNETIC PROPERTIES OF Co2YZ(Y = Cr, Z = Al, Ga) TYPE HEUSLER COMPOUNDS: A FIRST PRINCIPLE STUDY. *International Journal of Modern Physics B*, **2012**, 26, 1250071	1.1	16
165	GGA + U and mBJ + U study of the optoelectronic, magnetic and thermoelectric properties of the SmAlO3 compound with spin□orbit coupling. *International Journal of Modern Physics B*, **2016**, 30, 1650078	1.1	16
164	Electronic, and thermoelectric properties of half-heusler compounds MCoSb (M = Ti, Zr, Hf): a first principles study. *Materials Research Express*, **2019**, 6, 066307	1.7	15
163	Structural, electronic and magnetic properties of new full Heusler alloys Rh2CrZ (Z = Al, Ga, In): First-principles calculations. *Chinese Journal of Physics*, **2019**, 59, 281-290	3.5	15
162	Electronic, magnetic, optical and thermoelectric properties of CaCr Ni OsO double perovskites.. *RSC Advances*, **2020**, 10, 16179-16186	3.7	15
161	Thermoelectric properties of tetragonal half-Heusler compounds, TiXSb (X□=□Ge, Si): A probe from Density Functional Theory (DFT). *Journal of Alloys and Compounds*, **2017**, 726, 1155-1160	5.7	15
160	An investigation of semiconducting behavior in the minority spin of Co2CrZ (Z = Ga, Ge, As): LSDA and LSDA + U method. *Journal of Alloys and Compounds*, **2012**, 542, 257-263	5.7	15
159	Ground state calculation of the electronic structure and magnetic properties of Co2VAl: a local spin density approximation with exchange correlation potential study. *Physica Scripta*, **2012**, 86, 045702	2.6	15
158	Band gap modulation of mono and bi-layer hexagonal ZnS under transverse electric field and bi-axial strain: A first principles study. *Physica B: Condensed Matter*, **2018**, 531, 90-94	2.8	15
157	Electronic, magnetic and structural properties of the filled skutterudite EuFe4P12: LSDA and LSDA+U calculation. *Physica B: Condensed Matter*, **2013**, 427, 31-36	2.8	14
156	Solubility of Crystalline Calcium Isosaccharinate. *Journal of Solution Chemistry*, **1998**, 27, 1109-1122	1.8	14
155	First-principles calculations of rare earth (RE=Tm, Yb, Ce) doped ZnO: Structural, optoelectronic, magnetic, and electrical properties. *Vacuum*, **2020**, 181, 109603	3.7	14
154	A theoretical analysis of elastic and optical properties of half Heusler MCoSb (M=Ti, Zr and Hf). *Heliyon*, **2019**, 5, e01155	3.6	13
153	First principles study of the electronic and magnetic properties of semi-Heusler alloys NiXSb (X=Ti, V, Cr and Mn). *Journal of Alloys and Compounds*, **2011**, 509, 9742-9752	5.7	13
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150	Electronic and optical properties of 2D monolayer (ML) MoS2 with vacancy defect at S sites. *Nano Structures Nano Objects*, **2020**, 21, 100404	5.6	12
149	Spin-orbit coupling effect on electronic, optical, and thermoelectric properties of Janus GaSSe.. *RSC Advances*, **2020**, 10, 44785-44792	3.7	12
148	FP-LAPW calculations of the elastic, electronic and thermoelectric properties of the filled skutterudite CeRu4Sb12. *Journal of Solid State Chemistry*, **2016**, 240, 126-132	3.3	12
147	Electronic, optical and thermoelectric properties of PrMO3 (M = Al, Ga, In) from first-principles calculations. *RSC Advances*, **2016**, 6, 59988-59997	3.7	11
146	A comprehensive first-principles computational study on the physical properties of lutetium aluminum perovskite LuAlO3. *Materials Chemistry and Physics*, **2020**, 250, 123148	4.4	11
145	Hexagonal boron nitride (h-BN) nanosheet as a potential hydrogen adsorption material: A density functional theory (DFT) study. *Surfaces and Interfaces*, **2021**, 24, 101043	4.1	11
144	Compensated half metallicity in osmium double perovskite driven by doping effects. *Materials Research Express*, **2016**, 3, 106107	1.7	11
143	Theoretical investigation of the structural, electronic and thermodynamic properties of cubic and orthorhombic XZrS3 (X = Ba,Sr,Ca) compounds. *Journal of Computational Electronics*, **2019**, 18, 415-427	1.8	11
142	First-principles investigation of structural, elastic, thermodynamic, electronic and optical properties of lead-free double perovskites halides: Cs2LiYX6 (X = Br, I). *Materials Chemistry and Physics*, **2021**, 258, 123945	4.4	11
141	Electronic, optical and thermoelectric properties of bulk and surface (001) CuInTe 2 : A first principles study. *Journal of Alloys and Compounds*, **2017**, 699, 1003-1011	5.7	10
140	Effects of electron-correlation, spin-orbit coupling, and modified Becke-Johnson potential in double perovskites SrLaBB?O6(B = Ni, Fe; B? = Os, Ru). *Computational Materials Science*, **2019**, 170, 109168	3.3	10
139	Room-temperature ferrimagnetism of anti-site-disordered Ca2MnOsO6. *Physical Review Materials*, **2019**, 3,	3.2	10
138	An ab initio study of filled skutterudites ROs4P12 (R = Sm, Eu and Gd). *Phase Transitions*, **2015**, 88, 1062-1073	1.9	9
137	Electronic and magnetic properties of SmCrSb3 and GdCrSb3: A first principles study. *Journal of Magnetism and Magnetic Materials*, **2011**, 323, 2883-2887	2.8	9
136	Electronic and optical properties of bulk and surface of CsPbBr inorganic halide perovskite a first principles DFT 1/2 approach. *Scientific Reports*, **2021**, 11, 20622	4.9	9
135	Electronic, optical, and thermoelectric properties of Janus In-based monochalcogenides. *Journal of Physics Condensed Matter*, **2021**, 33,	1.8	9
134	Induced ferromagnetism in bilayer hexagonal Boron Nitride (h-BN) on vacancy defects at B and N sites. *Physica E: Low-Dimensional Systems and Nanostructures*, **2021**, 126, 114436	3	9

133	Half metallic ferromagnetism in tri-layered perovskites Sr4T3O10(T = Co, Rh). *Journal of Applied Physics*, **2015**, 117, 063903	2.5	8
132	Effect of Image Force on Tunneling Current for Ultra Thin Oxide Layer Based Metal Oxide Semiconductor Devices. *Nanoscience and Nanotechnology Letters*, **2015**, 7, 331-333	0.8	8
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130	Electronic, magnetic and optical properties of monolayer (ML) hexagonal ZnSe on vacancy defects at Zn sites from DFT-1/2 approach. *Vacuum*, **2020**, 182, 109597	3.7	8
129	Induced magnetic states upon electron□hole injection at B and N sites of hexagonal boron nitride bilayer: A density functional theory study. *International Journal of Quantum Chemistry*, **2021**, 121, e26680	2.1	8
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126	Structural, electronic, optical, thermodynamic and elastic properties of the zinc-blende AlxIn1-xN ternary alloys: A first principles calculations. *Journal of Physics and Chemistry of Solids*, **2018**, 119, 36-49	3.9	7
125	Analysis of Interface Charge Densities for High-k Dielectric Materials based Metal Oxide Semiconductor Devices. *International Journal of Nanoscience*, **2016**, 15, 1660011	0.6	7
124	Strain dependence of electronic properties and effective masses of monolayer ZnO from density functional theory **2019**,		7
123	Study of the Fe2CoAl heusler alloy films growth on the R-plane sapphire substrate by scanning probe microscopy. *Ferroelectrics*, **2019**, 541, 79-92	0.6	7
122	Electronic and magnetic properties of a full-Heusler alloy Co2CrGe: a first-principles study. *Journal of Theoretical and Applied Physics*, **2013**, 7, 1	1.4	7
121	Structural, electronic, magnetic and optical properties of neodymium chalcogenides using LSDA+Umethod. *Journal of Semiconductors*, **2012**, 33, 082001	2.3	7
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119	Predictions on structural, electronic, optical and thermal properties of lithium niobate via first-principle computations. *Philosophical Magazine*, **2020**, 100, 1150-1171	1.6	6
118	Promising optoelectronic response of 2D monolayer MoS2: A first principles study. *Chemical Physics* , **2020**, 538, 110824	2.3	6
117	Electronic structure and x-ray spectroscopy of Cu2MnAl1□Gax. *Journal of Applied Physics*, **2018**, 123, 161509	2.5	6
116	Origin of the optical anisotropy and the electronic structure of Ru-based double perovskite oxides: DFT and XPS studies. *RSC Advances*, **2017**, 7, 43531-43539	3.7	6

115	Electronic structure and thermoelectricity of filled skutterudite EuRu4As12: a DFT calculation. *Indian Journal of Physics*, **2017**, 91, 17-23	1.4	6
114	Electronic, magnetic, optical and transport properties of wurtzite-GaN doped with rare earth (RE= Pm, Sm, and Eu): First principles approach. *Surfaces and Interfaces*, **2021**, 24, 101051	4.1	6
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112	A first principles study of Nd doped cubic LaAlO3 perovskite: mBJ+U study. *Journal of Magnetism and Magnetic Materials*, **2016**, 417, 313-320	2.8	6
111	Electronic and thermoelectric properties of chalcopyrite compounds Cu2(XY)S4 (X = Zn, Cd and Y = Sn, Pb): first-principles study. *Indian Journal of Physics*, **2021**, 95, 281-287	1.4	6
110	The electronic and thermoelectric properties of a d2/d0type tetragonal half-Heusler compound, HfSiSb: a FP-LAPW method. *Materials Research Express*, **2017**, 4, 105506	1.7	5
109	Theoretical investigation of the structural stabilities, optoelectronic properties and thermodynamic characteristics of GaPxSb1⊠ ternary alloys. *Indian Journal of Physics*, **2018**, 92, 705-714	1.4	5
108	Electronic and optical properties of double perovskite Ba2VMoO6: FP-LAPW study **2018**,		5
107	Computational investigations on band structure and electronic features of chromium-based carbides and nitride Cr3PX (X⊠⊠C and N) through the FP-APW+LO approach. *Superlattices and Microstructures*, **2017**, 109, 1-12	2.8	5
106	Pressure dependent half-metallic ferromagnetism in inverse Heusler alloy FeCoAl: a DFT+U calculations.. *RSC Advances*, **2020**, 10, 44633-44640	3.7	5
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104	Re-entrant spin reorientation transition and Griffiths-like phase in antiferromagnetic TbFe0.5Cr0.5O3. *Physical Review B*, **2020**, 102,	3.3	5
103	FP-LAPW study of energy bands and optical properties of the filled skutterudite (hbox {CeRu}_{4}hbox {As}_{12}) with spin⊠orbit coupling. *Journal of Computational Electronics*, **2016**, 15, 721-728	1.8	5
102	Conductance Study of Aerosol-OT in Binary Mixed Solvents of Short-Chain Alcohol⊠Water Systems at Various Temperatures. *Journal of Chemical & Engineering Data*, **2021**, 66, 65-78	2.8	5
101	First-principles calculations of optoelectronic properties of CaO: Eu+2 (SrO: Eu+2) for energy applications. *International Journal of Modern Physics B*, **2018**, 32, 1850333	1.1	5
100	Evidence of two-dimensional flat band at the surface of antiferromagnetic kagome metal FeSn. *Nature Communications*, **2021**, 12, 5345	17.4	5
99	Effect of Fe-Ru doping in the electronic and thermoelectric properties of new filled skutterudite Ba(Fe,Ru)4As12. *Journal of Applied Physics*, **2017**, 121, 055103	2.5	4
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97	CeOs4As12: a hybridized gap semiconductor. *Indian Journal of Physics*, **2019**, 93, 1419-1425	1.4	4
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95	Interface Charge Density Measurement for Ultra Thin ZrO2 Material Based MOS Devices Using Conductance Method. *Procedia Computer Science*, **2015**, 57, 761-765	1.6	4
94	(Li,F) co-doped ZnO: Optoelectronic devices applications. *Superlattices and Microstructures*, **2020**, 145, 106645	2.8	4
93	Electronic and Piezoelectric properties of half-Heusler compounds: A first principles study. *Journal of Physics: Conference Series*, **2016**, 765, 012005	0.3	4
92	Energy band structure, elastic and optical constants of the filled skutterudite CeRu4As12. *Materials Science in Semiconductor Processing*, **2016**, 46, 10-16	4.3	4
91	Analysis of Interface Charge Using Capacitance-Voltage Method for Ultra Thin HfO2 Gate Dielectric Based MOS Devices. *Procedia Computer Science*, **2015**, 57, 757-760	1.6	4
90	Studying structural, electronic and optical properties of zinc-blende Ga1−xAlxP at normal and under pressure by means of first principle. *Materials Research Express*, **2015**, 2, 105904	1.7	4
89	Electronic and optical properties of CuInTe2. *Journal of Physics: Conference Series*, **2016**, 765, 012008	0.3	4
88	First principle study on pressure-induced electronic structure and elastic properties of indium phosphide (InP). *Indian Journal of Physics*, **2015**, 89, 1265-1271	1.4	3
87	Insight into the structural, electronic and elastic properties of AInQ2 (A: K, Rb and Q: S, Se, Te) layered structures from first-principles calculations. *Chinese Journal of Physics*, **2018**, 56, 1074-1088	3.5	3
86	A systematic study of LaAlO3 with variation of Nd doping, case of band gap tuning: A first principles method. *Modern Physics Letters B*, **2016**, 30, 1650028	1.6	3
85	Investigation of elastic and optical properties of EuFe4P12 by first principles calculation. *Indian Journal of Physics*, **2015**, 89, 797-801	1.4	3
84	Magnetic and electronic properties of half-metallic NiTbSb: a first principles study. *Indian Journal of Physics*, **2012**, 86, 301-305	1.4	3
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82	First principles study of the electronic and optical properties of SbTaO4. *Physica B: Condensed Matter*, **2011**, 406, 3454-3457	2.8	3
81	A First Principle Calculation of Full-Heusler Alloy Co2TiAl: LSDA+U Method **2012**, 2012, 1-5		3
80	Thorium reactions in borosilicate-glass/water systems. *Radiochimica Acta*, **2005**, 93,	1.9	3

79	Band-gap engineering of La 1−x Nd x AlO 3 (x = 0, 0.25, 0.50, 0.75, 1) perovskite using density functional theory: A modified Becke Johnson potential study. *Chinese Physics B*, **2016**, 25, 067101	1.2	3
78	SnCmonolayer with transition metal adatom for gas sensing: a density functional theory studies. *Nanotechnology*, **2021**, 32,	3.4	3
77	Investigation of half-metallicity of GeKMg and SnKMg by Using mBJ potential method. *Journal of Physics: Conference Series*, **2016**, 765, 012018	0.3	3
76	Outstanding elastic, electronic, transport and optical properties of a novel layered material CF: first-principles study.. *RSC Advances*, **2021**, 11, 23280-23287	3.7	3
75	Study of electronic and mechanical properties of single walled Carbon nanotube (SWCNT) via substitutional Boron doping in zigzag and armchair pattern. *Surfaces and Interfaces*, **2022**, 29, 101815	4.1	3
74	Electronic and optical properties of cubic bulk and ultrathin surface [001] slab of CsPbBr3. *Surfaces and Interfaces*, **2022**, 30, 101829	4.1	3
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72	Ferromagnetic half-metallicity in half-Heusler AuMnSn:Te Alloy. *Materials Research Express*, **2020**, 7, 076519	1.9	2
71	The Weak 3D Topological Insulator Bi Rh Sn I. *Chemistry - A European Journal*, **2020**, 26, 15549-15557	4.8	2
70	Preparation and characterization of (CuInTe2)1-x(TaTe)x solid solutions (0. *Journal of Alloys and Compounds*, **2018**, 747, 176-188	5.7	2
69	Effect of Si and Ge Surface Doping on the Be2C Monolayer: Case Study on Electrical and Optical Properties. *Silicon*, **2018**, 10, 1893-1902	2.4	2
68	Band Structure Simulations of the Structural, Electronic, Magnetic, and Half-Metallic Features of the Ti 2 CoAl1− Sn x (x = 0, 0.25, 0.50, 0.75, 1) Heusler Alloys. *Journal of Superconductivity and Novel Magnetism*, **2016**, 29, 3193-3199	1.5	2
67	First principles phase transition, elastic properties and electronic structure calculations for cadmium telluride under induced pressure: density functional theory, LDA, GGA and modified Becke−ohnson potential. *Materials Research Express*, **2016**, 3, 015901	1.7	2
66	A First Principles Calculation of Ferromagnetic EuFe4Sb12. *Physics Procedia*, **2014**, 54, 127-131		2
65	Low-temperature synthesis and particle size effect on photoluminescence of YVO4:Eu nanocrystals. *Journal of Experimental Nanoscience*, **2013**, 8, 396-402	1.9	2
64	X-dependence of energy band structures and thermoelectricity of CeRu4X12 (X = P, As, Sb). *Journal of Materials Science*, **2017**, 52, 1511-1522	4.3	2
63	A Theoretical Study of Bulk Tungsten (W) Based on Momentum Transfer (q-Dependent). *Advances in Optics*, **2014**, 2014, 1-9		2
62	A First Principle Study of Co2CrZ (Z=In, Sn, Sb) Based on FP-LAPW Method. *Journal of Superconductivity and Novel Magnetism*, **2013**, 26, 3507-3513	1.5	2

61	Ground state study of half-metallic ferromagnetism in the half-Heusler compound Gekca using density functional theory **2013**,		2
60	Electronic and magnetic properties of NdCrSb3: A first principles study. *Physica B: Condensed Matter*, **2011**, 406, 1862-1864	2.8	2
59	Ground state study of Electronic and Magnetic Properties of Co2MnZ (Z = Ge, Sn) type Heusler Compounds : A first Principle Study. *Journal of Physics: Conference Series*, **2012**, 377, 012074	0.3	2
58	A Comparative Study of 1D Monatomic Fe-chain and 3D Fe-bulk within the Density Functional Theory (DFT). *Nanoscience and Nanoengineering*, **2016**, 4, 52-57		2
57	N-doped direction-dependent electronic and mechanical properties of single-walled carbon nanotube (SWCNT) from a first-principles density functional theory (DFT) and MD-simulation.. *Journal of Molecular Graphics and Modelling*, **2021**, 111, 108111	2.8	2
56	Elastic Properties and Electronic Structures of Pressure Induced Zinc Sulphide (ZnS): A Density Functional Theory Study. *Advanced Science Letters*, **2015**, 21, 2906-2910	0.1	2
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