Bachir Bouhafs

List of Publications by Citations

183 papers	3,307 citations	31 h-index	48 g-index
185 ext. papers	3,641 ext. citations	2.4 avg, IF	5.09 L-index

#	Paper	IF	Citations
183	FP-LAPW investigations of electronic structure and bonding mechanism of NbC and NbN compounds. *Physica B: Condensed Matter*, **2003**, 325, 46-56	2.8	103
182	Full potential calculation of structural, electronic and elastic properties of alkaline earth oxides MgO, CaO and SrO. *Physica B: Condensed Matter*, **2004**, 344, 334-342	2.8	102
181	First-principles investigation of lattice constants and bowing parameters in wurtzite AlxGa1−xN, InxGa1−xN and InxAl1−xN alloys. *Semiconductor Science and Technology*, **2003**, 18, 850-856	1.8	101
180	First-principles elastic constants and electronic structure of BP, BAs, and BSb. *Physica Status Solidi (B): Basic Research*, **2004**, 241, 2881-2885	1.3	95
179	Molecular-dynamics simulation of structural and thermodynamic properties of boron nitride. *Journal of Physics Condensed Matter*, **1998**, 10, 4975-4984	1.8	84
178	First-principle calculations of structural, electronic and optical properties of BaTiO3 and BaZrO3 under hydrostatic pressure. *Solid State Communications*, **2005**, 136, 120-125	1.6	83
177	First-principles elastic constants and electronic structure of beryllium chalcogenides BeS, BeSe and BeTe. *Computational Materials Science*, **2007**, 38, 609-617	3.2	82
176	First-principle study of structural, electronic and elastic properties of SrS, SrSe and SrTe under pressure. *Physica B: Condensed Matter*, **2003**, 339, 208-215	2.8	79
175	First-principles calculations on the electronic structure of TiCxN1−x, ZrxNb1−xC and HfCxN1−x alloys. *Materials Chemistry and Physics*, **2005**, 91, 108-115	4.4	79
174	Trends in band-gap pressure coefficients in boron compounds BP, BAs, and BSb. *Journal of Physics Condensed Matter*, **2000**, 12, 5655-5668	1.8	77
173	The electronic structure of wurtzite and zincblende AlN: anab initiocomparative study. *New Journal of Physics*, **2002**, 4, 64-64	2.9	74
172	Calculation of structural, optical and electronic properties of ZnS, ZnSe, MgS, MgSe and their quaternary alloy Mg1−xZnxSySe1−y. *Materials Science and Engineering B: Solid-State Materials for Advanced Technology*, **2003**, 100, 163-171	3.1	73
171	Structural, electronic, elastic and high-pressure properties of some alkaline-earth chalcogenides: An ab initio study. *Physica B: Condensed Matter*, **2006**, 371, 12-19	2.8	64
170	First-principles calculations of the elastic, electronic, and optical properties of the filled skutterudites CeFe4P12 and ThFe4P12. *Physical Review B*, **2007**, 75,	3.3	62
169	Full-potential calculations of structural, elastic and electronic properties of MgAl2O4 and ZnAl2O4 compounds. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2005**, 344, 271-279	2.3	58
168	First-principles calculations of vacancy effects on structural and electronic properties of TiCxand TiNx. *Journal of Physics Condensed Matter*, **2002**, 14, 10237-10249	1.8	55
167	Structural and electronic properties of the Laves phase based on rare earth type BaM2 (M=Rh, Pd, Pt). *Results in Physics*, **2012**, 2, 58-65	3.7	54

166	Half-metallic ferromagnetism in PrMnO3 perovskite from first principles calculations. *Solid State Communications*, **2013**, 168, 6-10	1.6	50
165	First-principles study of structural and electronic properties of BSb. *Journal of Physics Condensed Matter*, **1998**, 10, 7995-8006	1.8	48
164	Optical properties of BP, BAs and BSb compounds under hydrostatic pressure. *Physica B: Condensed Matter*, **2005**, 367, 195-204	2.8	46
163	Structural, electronic and optical calculations of Cu(In,Ga)Se2 ternary chalcopyrites. *Physica Status Solidi (B): Basic Research*, **2004**, 241, 2516-2528	1.3	42
162	Competition between the ionic and covalent character in the series of boron compounds BP, BAs, and BSb. *Journal of Physics Condensed Matter*, **1999**, 11, 5781-5796	1.8	41
161	First-principle study of magnetic, elastic and thermal properties of full Heusler Co2MnSi. *Intermetallics*, **2014**, 44, 26-30	3.5	39
160	The ground state and the bonding properties of the hypothetical cubic zinc-blende-like GeC and SnC compounds. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2001**, 282, 299-308	2.3	39
159	Electronic and optical properties of copper halides mixed crystal CuCl1−xIx. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **1998**, 240, 257-264	2.3	38
158	Electronic and Magnetic Properties of Co2CrGa1− Si x Heusler Alloys. *Journal of Superconductivity and Novel Magnetism*, **2017**, 30, 421-424	1.5	37
157	First principles calculations of structural, electronic and optical properties of BaLiF3. *Computational Materials Science*, **2009**, 44, 1265-1271	3.2	36
156	First-principles study of bonding mechanisms in the series of Ti, V, Cr, Mo, and their carbides and nitrides. *Physica B: Condensed Matter*, **2005**, 358, 63-71	2.8	34
155	First-principles calculations of optical properties of GeC, SnC and GeSn under hydrostatic pressure. *Physica B: Condensed Matter*, **2005**, 355, 392-400	2.8	32
154	Structural, elastic, electronic and thermodynamic properties of uranium filled skutterudites UFe4P12: First principle method. *Materials Science in Semiconductor Processing*, **2014**, 27, 368-379	4.3	31
153	First-principles calculations of the structural, electronic and optical properties of and. *Physica B: Condensed Matter*, **2005**, 367, 142-151	2.8	31
152	Structural, electronic and optical properties of fluorite-type compounds. *European Physical Journal B*, **2005**, 47, 63-70	1.2	30
151	First-principles calculations of the structural, electronic and optical properties of IIAIV antifluorite compounds. *Physica Status Solidi (B): Basic Research*, **2005**, 242, 2022-2032	1.3	30
150	Pressure dependence of energy band gaps for AlxGa1 -xN, InxGa1 -xN and InxAl1 -xN. *New Journal of Physics*, **2002**, 4, 94-94	2.9	30
149	Stability and electronic properties of ZnxCd1−xO alloys. *Materials Chemistry and Physics*, **2010**, 120, 98-103	4.4	29

148	Gd impurities effect on (hbox {Co}_{2}hbox {CrSi}) alloy: first-principle calculations. *Bulletin of Materials Science*, **2018**, 41, 1	1.7	28
147	Unusual structural and electronic properties of SnxGe1 alloys. *Physica Status Solidi (B): Basic Research*, **2003**, 240, 116-119	1.3	28
146	Vacancy defects in strontium titanate: Ab initio calculation. *Computational Materials Science*, **2010**, 49, 904-909	3.2	26
145	FP-LAPW investigation of structural, electronic, and thermodynamic properties of Al3V and Al3Ti compounds. *Physica B: Condensed Matter*, **2010**, 405, 4045-4050	2.8	26
144	Full-potential electronic structure of Hf2AlC and Hf2AlN. *Acta Materialia*, **2007**, 55, 4161-4165	8.4	26
143	Theoretical analysis of d electron effects on the electronic properties of wurtzite and zincblende GaN. *Physica Status Solidi (B): Basic Research*, **2003**, 236, 61-81	1.3	26
142	Full-relativistic calculation of electronic structure of Zr2AlC and Zr2AlN. *Solid State Communications* , **2006**, 139, 485-489	1.6	25
141	First-Principles Calculations of Optical Properties of AlN, GaN, and InN Compounds under Hydrostatic Pressure. *Physica Status Solidi (B): Basic Research*, **2001**, 228, 457-460	1.3	24
140	Structural, elastic, electronic and thermodynamic properties of the filled skutterudite CeOs4Sb12 determined by density functional theory. *Materials Science in Semiconductor Processing*, **2013**, 16, 1508-1516	4.3	23
139	First-principles calculations of the optical band-gaps of ZnxCd1O alloys. *Superlattices and Microstructures*, **2007**, 42, 165-171	2.8	23
138	Generalized gradient calculations of magneto-electronic properties for diluted magnetic semiconductors ZnMnS and ZnMnSe. *Physica B: Condensed Matter*, **2008**, 403, 3452-3458	2.8	23
137	Structural, elastic, electronic and thermodynamic investigations of neptunium chalcogenides: First-principles calculations. *Chinese Journal of Physics*, **2016**, 54, 33-41	3.5	23
136	Effect of Coulomb interactions and Hartree-Fock exchange on structural, elastic, optoelectronic and magnetic properties of Co2MnSi Heusler: A comparative study. *Journal of Magnetism and Magnetic Materials*, **2016**, 419, 74-83	2.8	22
135	The spin effect in zinc-blende Cd0.5Mn0.5Te and Zn0.5Mn0.5Te diluted magnetic semiconductors: FP-LAPW study. *Physica B: Condensed Matter*, **2010**, 405, 625-631	2.8	22
134	First-principles calculations of the structural, electronic and optical properties of cubic BxGa1As alloys. *Physica B: Condensed Matter*, **2012**, 407, 1292-1300	2.8	20
133	Structural and electronic properties calculations of BexZn1Se alloy. *Materials Science in Semiconductor Processing*, **2007**, 10, 6-13	4.3	20
132	First-principles study of cubic AlxGa1N alloys. *Computational Materials Science*, **2005**, 33, 136-140	3.2	20
131	Semiconductor behavior of halide perovskites AGeX3 (A = K, Rb and Cs; X = F, Cl and Br): first-principles calculations. *Indian Journal of Physics*, **2020**, 94, 455-467	1.4	20

130	Energy band structure calculation of GexSn1− and SixSn1− alloys. *Infrared Physics and Technology*, **1995**, 36, 967-972	2.7	19
129	Structure and magnetic properties of the 3d transition-metal mono-borides TMB (TM=Mn, Fe, Co) under pressures. *Journal of Magnetism and Magnetic Materials*, **2014**, 365, 23-30	2.8	18
128	First-principles investigation on structural, elastic, electronic and thermodynamic properties of filled skutterudite PrFe4P12 compound for thermoelectric applications. *Molecular Simulation*, **2014**, 40, 1236-1243	2	18
127	Electronic structure of AlxGa1 −xAs and GaPxAs1 −x alloys modified virtual crystal approximation calculation using sp3s* band structures. *Materials Science and Engineering B: Solid-State Materials for Advanced Technology*, **1996**, 41, 304-309	3.1	18
126	Half-Metallic Ferromagnetism in Double Perovskite Ca2CoMoO6 Compound: DFT+U Calculations. *Spin*, **2017**, 07, 1750009	1.3	17
125	First-Principles Calculations of Structural, Electronic, Optical, and Thermodynamic Properties of CdS, CdTe and Their Ternary Alloys CdS1-xTex(0.0≤x≤1.0). *Acta Physica Polonica A*, **2014**, 125, 1110-1117	0.6	17
124	A theoretical investigation of ZnOx S1− alloy band structure. *Physica Status Solidi (B): Basic Research*, **2007**, 244, 1560-1566	1.3	17
123	Meta-GGA calculation of the electronic structure of group IIIV nitrides. *Physica Status Solidi (B): Basic Research*, **2006**, 243, 1577-1582	1.3	17
122	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
121	Electronic structure and magnetism of cubic Ga1−EuxN and Al1−EuxN using the LSDA + U approach. *Computational Materials Science*, **2010**, 48, 743-748	3.2	16
120	ELECTRONIC AND OPTICAL PROPERTIES OF BaO, BaS, BaSe, BaTe AND BaPo COMPOUNDS UNDER HYDROSTATIC PRESSURE. *Modern Physics Letters B*, **2009**, 23, 3065-3079	1.6	16
119	Theoretical investigation of electronic structure of PbSxTe1− and PbSexTe1− alloys. *Materials Chemistry and Physics*, **2009**, 114, 650-655	4.4	16
118	First principles calculations of structural, electronic and optical properties of BAs1−Px alloy. *Physics Procedia*, **2009**, 2, 933-940		16
117	GGA + U Study of Electronic and Magnetic Properties of Pr(Fe/Cr)O3 Cubic Perovskites. *Journal of Superconductivity and Novel Magnetism*, **2017**, 30, 2581-2590	1.5	15
116	First-principle study of structural, elastic and electronic properties of Th monopnictides. *Journal of Nuclear Materials*, **2014**, 454, 186-191	3.3	15
115	Electronic properties and stability of ZnO from computational study. *Physica B: Condensed Matter*, **2008**, 403, 3154-3158	2.8	15
114	Full potential linearized augmented plane wave calculations of positronic and electronic charge densities of zinc-blende AlN, InN and their alloy Al0.5In0.5N. *Journal of Solid State Chemistry*, **2005**, 178, 2117-2127	3.3	15
113	Investigated electronic structure and magnetic ordering of rare earth impurities (Eu, Gd) in ZnO. *International Journal of Modern Physics B*, **2016**, 30, 1650225	1.1	14

112	Half-metallic ferromagnetism in ZnCrTe and CdCrTe: Ab initio study. *Computational Materials Science*, **2011**, 50, 2785-2792	3.2	13
111	First principles calculation of electronic structure, bonding and chemical stability of TiB2, NbB2 and their ternary alloy Ti0.5Nb0.5B2. *Physica B: Condensed Matter*, **2010**, 405, 540-546	2.8	13
110	Theoretical analysis of the spin effect on the electronic and magnetic properties of the calcium manganese oxide CaMnO3: GGA+U calculation. *Physica B: Condensed Matter*, **2010**, 405, 4595-4606	2.8	13
109	Theoretical analysis of disorder effects on electronic and optical properties in InGaAsP quaternary alloy. *Journal of Applied Physics*, **1997**, 82, 4923-4930	2.5	13
108	Electronic and Optical Properties of Copper Halide Mixed Crystals CuBr1−xIx. *Physica Status Solidi (B): Basic Research*, **1998**, 209, 339-352	1.3	13
107	Ab initio study of cubic PbSxSe1−x alloys. *Journal of Alloys and Compounds*, **2008**, 462, 135-141	5.7	13
106	First-principle calculations of electronic and positronic properties of AlGaAs2. *Physica B: Condensed Matter*, **2007**, 396, 169-176	2.8	13
105	Theoretical analysis of disorder effects on electronic and optical properties of the quaternary alloy In1−xGaxAsySb1−y epilayer on GaSb and InAs. *Physica Status Solidi (B): Basic Research*, **2003**, 238, 156-172	1.3	13
104	Optoelectronic properties of germanium iodide perovskites AGeI3 (A = K, Rb and Cs): first principles investigations. *Optical and Quantum Electronics*, **2019**, 51, 1	2.4	12
103	Ferromagnetism in RaBi with Zinc-Blende and Wurtzite Structures: Ab-initio Prediction. *Spin*, **2018**, 08, 1850008	1.3	11
102	Ab initio calculations of structural, elastic, and thermodynamic properties of HoX (X=N, O, S and Se). *Materials Science in Semiconductor Processing*, **2014**, 26, 205-217	4.3	11
101	First principles calculations of structural, electronic, thermodynamic and optical properties of BAs1 -xPxalloy. *Physica Scripta*, **2009**, 79, 045002	2.6	11
100	Ab initio studies of structural, elastic and electronic properties of ZrxNb1−xC and ZrxNb1−xN alloys. *Physica B: Condensed Matter*, **2010**, 405, 153-157	2.8	11
99	Empirical Pseudo-Potential Calculations in GaAs1−xNx and AlAs1−xNx Ordered Alloys. *Physica Status Solidi (B): Basic Research*, **1997**, 201, 117-134	1.3	11
98	Band structure calculations of Ga1 −xAlxAs, GaAs1 −xPx and AlAs under pressure. *Computational Materials Science*, **1995**, 3, 393-401	3.2	11
97	First-principles study of the electronic structure, magnetism, and phonon dispersions for CaX (X= C, N) compounds. *Computational Condensed Matter*, **2018**, 17, e00336	1.7	11
96	Structural, electronic and optical properties of cubic fluoroelpasolite Cs2NaYF6 by density functional theory. *Chinese Journal of Physics*, **2018**, 56, 1756-1763	3.5	11
95	Half metallic properties of the quaternary CuFe2GaSe4 chalcogenide compound. *Computational Materials Science*, **2014**, 85, 159-163	3.2	10

94	Spin-polarized calculations of electronic structures in ferromagnetic and antiferromagnetic Zn0.75TM0.25Se (TM=Cr, Fe, Co and Ni). *Journal of Magnetism and Magnetic Materials*, **2012**, 324, 2800-2805	2.8	10
93	First principle calculations of structural, electronic and thermodynamic properties of Al3(TixV1−x) alloy in D022 and L12 structures. *Solid State Sciences*, **2013**, 16, 1-5	3.4	10
92	Vacancy effects on structural and electronic properties of 4d transition-metal carbides. *Computational Materials Science*, **2009**, 44, 1071-1075	3.2	10
91	Interband transitions of wide-band-gap ternary pnictide BeCN2 in the chalcopyrite structure. *Physica Status Solidi (B): Basic Research*, **2004**, 241, 305-316	1.3	10
90	The electronic structure of CuCl. *Computational Materials Science*, **2001**, 20, 267-274	3.2	10
89	Electronic, Elastic, and Magnetic Properties of the Full-Heusler with the 4d Transition Metal Element, Co2YSi, Co2ZrSi, and Co2Y0.5Zr0.5Si: a First-Principle Study. *Journal of Superconductivity and Novel Magnetism*, **2016**, 29, 2311-2317	1.5	10
88	Spin-Polarized Calculations of Magnetic and Thermodynamic Properties of the Full-Heusler (mathrm{{Co}}_{2})MnZ (Z = Al, Ga). *International Journal of Thermophysics*, **2013**, 34, 507-520	2.1	9
87	First-principles study of electronic structure and magnetism of cubic Al1−xErxN using the LSDA+U approach. *Journal of Magnetism and Magnetic Materials*, **2011**, 323, 1174-1178	2.8	9
86	Electronic and optical properties of copper halides mixed crystal CuCl1−xBrx. *Journal of Physics and Chemistry of Solids*, **1998**, 59, 997-1007	3.9	9
85	Electronic structure and optical properties of (ZnSe)n(Si2)m (111) superlattices. *Journal of Applied Physics*, **2006**, 99, 043702	2.5	9
84	Ferromagnetism in 4H-GaN polytype doped by non-magnetic light elements Li, Be, B, C, O, F, Ne, Na, and Mg: Ab-initio study. *Journal of Magnetism and Magnetic Materials*, **2016**, 414, 153-157	2.8	9
83	Ab-Initio Prediction of Intrinsic Half-Metallicity in Binary Alkali Metal Chalcogenides: KX (X=S, Se and Te). *Spin*, **2018**, 08, 1850020	1.3	9
82	Full-potential study of d-electrons effects on the electronic structure of wurtzite and zinc-blende InN. *Physica Status Solidi (A) Applications and Materials Science*, **2006**, 203, 35-41	1.6	8
81	Insight into the structural, elastic and electronic properties of tetragonal inter-alkali metal chalcogenides CsNaX (X=S, Se, and Te) from first-principles calculations. *Materials Chemistry and Physics*, **2019**, 221, 125-137	4.4	8
80	Investigation of new d0 half-metallic full-heusler alloys N2BaX (X=Rb, Cs, Ca and Sr) using first-principle calculations. *Computational Condensed Matter*, **2019**, 19, e00371	1.7	7
79	Half-Metallic and Half-Semiconductor Gaps in Cr-Based Chalcogenides: DFT + U Calculations. *Journal of Superconductivity and Novel Magnetism*, **2019**, 32, 635-649	1.5	7
78	DFT + U studies of the electronic and optical properties of ReS2 mono-layer doped with lanthanide atoms. *Materials Research Express*, **2019**, 6, 106307	1.7	7
77	FP-LMTO method to calculate the structural, thermodynamic and optoelectronic properties of SixGe1−xC alloys. *Molecular Physics*, **2013**, 111, 3208-3217	1.7	7

76	The spin effect in zinc-blende CdEuS and CdEuSe: GGA and GGA+U studies. *Physica B: Condensed Matter*, **2012**, 407, 3639-3645	2.8	7
75	Electronic structure, optical and dielectric constant of compounds Indium-based: InAlP2, and InGaP2 in its chalcopyrite, CuPt and CuAu-I structures. *Materials Science in Semiconductor Processing* , **2013**, 16, 1454-1465	4.3	7
74	Electronic structure of cubic ErxGa1−xN using the LSDA+U approach. *Physica B: Condensed Matter*, **2008**, 403, 2702-2706	2.8	7
73	Realization of p-Type Conductivity in ZnO via Potassium Doping. *Acta Physica Polonica A*, **2016**, 129, 1155-1158	0.6	7
72	A datamining approach to predict the formation enthalpy for rare-earth dihydrides REH2 (RE = Ce,Pr,Dy). *International Journal of Hydrogen Energy*, **2016**, 41, 11254-11263	6.7	7
71	Rattling Heusler semiconductors: Thermoelectric properties: First-principles prediction. *Chinese Journal of Physics*, **2019**, 57, 195-210	3.5	7
70	First-Principles Studies of Structural, Electronic and Magnetic Properties of the CrS, CrSe and CrTe Compounds. *Spin*, **2018**, 08, 1850019	1.3	7
69	Thermodynamic, structural and electronic, properties of SnO2: By GGA and GGA + trans-blaha-modified Becke–Johnson (TB-mBJ) calculation. *Superlattices and Microstructures*, **2015**, 84, 80-90	2.8	6
68	Magnetic, Optoelectronic, and Thermodynamic Properties of Sr2CrXO6 (X = La and Y): Half-Metallic and Ferromagnetic Behavior. *Journal of Superconductivity and Novel Magnetism*, **2018**, 31, 3965-3979	1.5	6
67	Structural and elastic properties of TiN and AlN compounds: first-principles study. *Materials Science-Poland*, **2014**, 32, 220-227	0.6	6
66	Ferromagnetism in CdOX (X=Mn and N) with and without intrinsic point defects: A density functional theory. *Results in Physics*, **2013**, 3, 205-208	3.7	6
65	Structural Stability, Electronic and Magnetic Properties of (Ni1−xCox)2MnSn Quaternary Heusler Alloys. *Spin*, **2017**, 07, 1750010	1.3	6
64	Electronic structure, magnetic and thermal properties of Rh2MnZ (Z=Ge, Sn, Pb) compounds under pressure from ab-initio quasi-harmonic method. *Journal of Magnetism and Magnetic Materials*, **2014**, 371, 130-134	2.8	6
63	First-Principles Study of Ferromagnetism in Iron Chromite Spinels: FeCr2O4 and CrFe2O4. *Spin*, **2019**, 09, 1950014	1.3	5
62	First-Principles Study of the New Half-Metallic Ferromagnetic Quaternary-Heusler Alloys NaXNO (X=Ca, Sr, Ba). *Spin*, **2020**, 10, 2050022	1.3	5
61	Density functional theory studies of the SrC and SrN compounds. *Materials Chemistry and Physics*, **2019**, 237, 121875	4.4	5
60	Correlation effects on the electronic structure of Co2Mn0.5Fe0.5Si and Co2Mn0.5Gd0.5Si quaternary alloys. *Intermetallics*, **2013**, 37, 27-31	3.5	5
59	Pressure dependence of electronic properties in zinc-blende-like SiGe compound. *Journal of Physics and Chemistry of Solids*, **1998**, 59, 759-768	3.9	5

58	Ordering effects on the electronic structures of AlN/GaN, InN/GaN and InN/AlN superlattices. *Computational Materials Science*, **2005**, 33, 157-162	3.2	5
57	The large rotations theory of elasto-viscoplastic shells subjected to the dynamic and thermal loads. *Engineering Computations*, **2003**, 20, 366-389	1.4	5
56	Theoretical analysis of disorder effects on electronic and optical properties of the quaternary alloy Ga1−xAlxAsySb1−y. *Materials Chemistry and Physics*, **2002**, 74, 328-335	4.4	5
55	Electronic and mechanical properties of MgN compound: Prediction of stable half-metallic ferromagnet in NaCl and ZB phases. *Journal of Magnetism and Magnetic Materials*, **2018**, 466, 28-37	2.8	5
54	d0 Half-Metallic Ferromagnetism in GeNaZ (Z = Ca, Sr, and Ba) Ternary Half-Heusler Alloys: an Ab initio Investigation. *Journal of Superconductivity and Novel Magnetism*, **2020**, 33, 3121-3132	1.5	4
53	Electronic and magnetic properties of Fe2SiC. *European Physical Journal B*, **2014**, 87, 1	1.2	4
52	First-principles calculations of magnetic properties for CdCrO2 under pressure. *Journal of Magnetism and Magnetic Materials*, **2013**, 327, 76-78	2.8	4
51	Structural, electronic and energetic properties of silicon carbon alloys. *Physica B: Condensed Matter*, **2007**, 388, 167-173	2.8	4
50	Predictive study of electronic properties of silicon–carbon alloys. *Materials Science and Engineering B: Solid-State Materials for Advanced Technology*, **2005**, 122, 145-151	3.1	4
49	Tight-Binding Calculation of Electronic and Elastic Properties of Ge. *Physica Status Solidi (B): Basic Research*, **2000**, 217, 911-917	1.3	4
48	Predicted modifications in the direct and indirect gaps of Si. *Solid State Communications*, **1995**, 96, 245-250	1.6	4
47	Thermoelectric and Half-Metallic Behavior of the Novel Heusler Alloy RbCrC: Ab initio DFT Study. *Spin*, **2020**, 10, 2050029	1.3	4
46	Predicted dynamically stable new phase for CrO2 compound: DFT + U calculations. *Computational Condensed Matter*, **2019**, 21, e00400	1.7	3
45	Ab initio studies of the structural, electronic and magnetic properties of stannite CuFe2-III-VI4 (III = Al, Ga, In and VI = S, Se, Te) alloys. *Computational Condensed Matter*, **2020**, 23, e00459	1.7	3
44	Ab initio full-potential study of mechanical properties and magnetic phase stability of californium monopnictides (CfN and CfP). *Journal of Nuclear Materials*, **2016**, 478, 149-157	3.3	3
43	Structural and electronic properties of non-magnetic intermetallic YAuX (X = Ge and Si) in hexagonal and cubic phases. *Bulletin of Materials Science*, **2016**, 39, 195-200	1.7	3
42	Electronic structure and magnetic ordering in gadolinium-doped AlGaN from LSDA + U calculations. *International Journal of Computational Materials Science and Engineering*, **2018**, 07, 1850019	0.3	3
41	Ab-initio investigation of structural, electronic, magnetic, and thermodynamic properties of XPt3 (X=V, Cr, Mn, and Fe) intermetallic compounds. *Computational Condensed Matter*, **2018**, 16, e00328	1.7	3

40	First-principles prediction of structural and electronic properties of RTAsO (R=La, Gd and T=Co, Ni) compounds by LSDA+U calculations. *Physica B: Condensed Matter*, **2010**, 405, 3525-3531	2.8	3
39	First-Principles Calculation of Structural and Electronic Properties of Wurtzite AlxGa1−xN, InxGa1−xN, and InxAl1−xN Random Alloys. *Physica Status Solidi C: Current Topics in Solid State Physics*, **2003**, 315-319		3
38	Calculation of the electronic and elastic properties of carbon. *Journal of Physics Condensed Matter*, **1998**, 10, 3195-3200	1.8	3
37	Prediction of High Pressure Phase Transition in Al Compounds by the Ionicity Character. *Physica Status Solidi (B): Basic Research*, **1995**, 189, K5-K8	1.3	3
36	SnCmonolayer with transition metal adatom for gas sensing: a density functional theory studies. *Nanotechnology*, **2021**, 32,	3.4	3
35	Prediction of half-metallicity in the NaS, NaSe and NaTe alkali-metal chalcogenides using first principles. *International Journal of Computational Materials Science and Engineering*, **2018**, 07, 1850015	0.3	3
34	Ab-initio prediction of half-metallicity in Lithium chalcogenides compounds LiX (X=S, Se and Te) in zinc-blende and wurtzite structures. *Computational Condensed Matter*, **2018**, 16, e00318	1.7	3
33	Prediction of Half-Metallic Properties in Non-transition Metal-based Binary Compounds X Bi (X = Ba, Sr and Ca) with Zinc-Blende and Wurtzite Structures. *Journal of Superconductivity and Novel Magnetism*, **2018**, 31, 2767-2776	1.5	2
32	The effect of the correlation and exchange interactions on the electronic and magnetic properties of the hexagonal NiS using the onsite exact exchange/hybrid functionals. *Physica B: Condensed Matter*, **2017**, 526, 89-95	2.8	2
31	First-principles prediction of insulating antiferromagnet in ordered double-perovskite Ca2MnMoO6 compound. *International Journal of Computational Materials Science and Engineering*, **2017**, 06, 1750027	0.3	2
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