Bachir Bouhafs

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/2447437/publications.pdf

Version: 2024-02-01

185 papers	4,031 citations	126708 33 h-index	161609 54 g-index
185 all docs	185 docs citations	185 times ranked	2913 citing authors

#	Article	IF	Citations
1	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.	1.3	115
2	FP-LAPW investigations of electronic structure and bonding mechanism of NbC and NbN compounds. Physica B: Condensed Matter, 2003, 325, 46-56.	1.3	114
3	First-principles investigation of lattice constants and bowing parameters in wurtzite AlxGa1ÂxN, InxGa1ÂxN and InxAl1ÂxN alloys. Semiconductor Science and Technology, 2003, 18, 850-856.	1.0	109
4	First-principles elastic constants and electronic structure of BP, BAs, and BSb. Physica Status Solidi (B): Basic Research, 2004, 241, 2881-2885.	0.7	108
5	First-principle calculations of structural, electronic and optical properties of BaTiO3 and BaZrO3 under hydrostatic pressure. Solid State Communications, 2005, 136, 120-125.	0.9	104
6	First-principle study of structural, electronic and elastic properties of SrS, SrSe and SrTe under pressure. Physica B: Condensed Matter, 2003, 339, 208-215.	1.3	92
7	Molecular-dynamics simulation of structural and thermodynamic properties of boron nitride. Journal of Physics Condensed Matter, 1998, 10, 4975-4984.	0.7	91
8	First-principles calculations on the electronic structure of TiCxN1â^'x, ZrxNb1â^'xC and HfCxN1â^'x alloys. Materials Chemistry and Physics, 2005, 91, 108-115.	2.0	90
9	Trends in band-gap pressure coefficients in boron compounds BP, BAs, and BSb. Journal of Physics Condensed Matter, 2000, 12, 5655-5668.	0.7	89
10	First-principles elastic constants and electronic structure of beryllium chalcogenides BeS, BeSe and BeTe. Computational Materials Science, 2007, 38, 609-617.	1.4	89
11	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.	2.0	89
12	Calculation of structural, optical and electronic properties of ZnS, ZnSe, MgS, MgSe and their quaternary alloy Mg1â^'xZnxSySe1â^'y. Materials Science and Engineering B: Solid-State Materials for Advanced Technology, 2003, 100, 163-171.	1.7	83
13	The electronic structure of wurtzite and zincblende AlN: anab initiocomparative study. New Journal of Physics, 2002, 4, 64-64.	1.2	78
14	Gd impurities effect on $$hbox {Co}_{2}hbox {CrSi}$$ Co 2 CrSi alloy: first-principle calculations. Bulletin of Materials Science, 2018, 41, 1.	0.8	74
15	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.	0.9	73
16	Structural, electronic, elastic and high-pressure properties of some alkaline-earth chalcogenides: An ab initio study. Physica B: Condensed Matter, 2006, 371, 12-19.	1.3	69
17	Half-metallic ferromagnetism in PrMnO3 perovskite from first principles calculations. Solid State Communications, 2013, 168, 6-10.	0.9	69
18	First-principles calculations of the elastic, electronic, and optical properties of the filled skutteruditesCeFe4P12andThFe4P12. Physical Review B, 2007, 75, .	1.1	66

#	Article	IF	Citations
19	First-principles calculations of vacancy effects on structural and electronic properties of TiCxand TiNx. Journal of Physics Condensed Matter, 2002, 14, 10237-10249.	0.7	65
20	First-principles study of structural and electronic properties of BSb. Journal of Physics Condensed Matter, 1998, 10, 7995-8006.	0.7	56
21	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.	0.7	53
22	Optical properties of BP, BAs and BSb compounds under hydrostatic pressure. Physica B: Condensed Matter, 2005, 367, 195-204.	1.3	51
23	First-principle study of magnetic, elastic and thermal properties of full Heusler Co2MnSi. Intermetallics, 2014, 44, 26-30.	1.8	51
24	Semiconductor behavior of halide perovskites AGeX3 (Aâ€‰=â€‰K, Rb and Cs; Xâ€‰=â€‰F, Cl and Br): first-principles calculations. Indian Journal of Physics, 2020, 94, 455-467.	0.9	51
25	Structural, elastic, electronic and thermodynamic properties of uranium filled skutterudites UFe4P12: First principle method. Materials Science in Semiconductor Processing, 2014, 27, 368-379.	1.9	50
26	Structural, electronic and optical calculations of Cu(In,Ga)Se2 ternary chalcopyrites. Physica Status Solidi (B): Basic Research, 2004, 241, 2516-2528.	0.7	47
27	First principles calculations of structural, electronic and optical properties of BaLiF3. Computational Materials Science, 2009, 44, 1265-1271.	1.4	47
28	Electronic and optical properties of copper halides mixed crystal CuCl1â^'xIx. Physics Letters, Section A: General, Atomic and Solid State Physics, 1998, 240, 257-264.	0.9	46
29	Electronic and Magnetic Properties of Co2CrGa1â^'x Si x Heusler Alloys. Journal of Superconductivity and Novel Magnetism, 2017, 30, 421-424.	0.8	46
30	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.	0.9	45
31	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.	1.3	38
32	First-principles calculations of the structural, electronic and optical properties of and. Physica B: Condensed Matter, 2005, 367, 142-151.	1.3	36
33	First-principles calculations of optical properties of GeC, SnC and GeSn under hydrostatic pressure. Physica B: Condensed Matter, 2005, 355, 392-400.	1.3	35
34	Pressure dependence of energy band gaps for AlxGa1 -xN, InxGa1 -xN and InxAl1 -xN. New Journal of Physics, 2002, 4, 94-94.	1.2	32
35	First-principles calculations of the structural, electronic and optical properties of IIA-IV antifluorite compounds. Physica Status Solidi (B): Basic Research, 2005, 242, 2022-2032.	0.7	32
36	FP-LAPW investigation of structural, electronic, and thermodynamic properties of Al3V and Al3Ti compounds. Physica B: Condensed Matter, 2010, 405, 4045-4050.	1.3	32

#	Article	IF	Citations
37	Structural, electronic and optical properties of fluorite-type compounds. European Physical Journal B, 2005, 47, 63-70.	0.6	31
38	Full-relativistic calculation of electronic structure of Zr2AlC and Zr2AlN. Solid State Communications, 2006, 139, 485-489.	0.9	30
39	Stability and electronic properties of ZnxCd1â^'xO alloys. Materials Chemistry and Physics, 2010, 120, 98-103.	2.0	30
40	Structural, elastic, electronic and thermodynamic investigations of neptunium chalcogenides: First-principles calculations. Chinese Journal of Physics, 2016, 54, 33-41.	2.0	30
41	Controlling the electronic and optical properties of HfS₂ mono-layers via lanthanide substitutional doping: a DFT+U study. RSC Advances, 2020, 10, 15670-15676.	1.7	30
42	Full-potential electronic structure of Hf2AlC and Hf2AlN. Acta Materialia, 2007, 55, 4161-4165.	3.8	29
43	Unusual structural and electronic properties of SnxGe1â^'x alloys. Physica Status Solidi (B): Basic Research, 2003, 240, 116-119.	0.7	28
44	Vacancy defects in strontium titanate: Ab initio calculation. Computational Materials Science, 2010, 49, 904-909.	1.4	28
45	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.	1.0	28
46	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.	1.9	27
47	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.	0.7	26
48	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.	0.7	26
49	Optoelectronic properties of germanium iodide perovskites AGeI3 (Aâ€‰=â€‰K, Rb and Cs): first principles investigations. Optical and Quantum Electronics, 2019, 51, 1.	1.5	26
50	Generalized gradient calculations of magneto-electronic properties for diluted magnetic semiconductors ZnMnS and ZnMnSe. Physica B: Condensed Matter, 2008, 403, 3452-3458.	1.3	25
51	First-principles calculations of the optical band-gaps of ZnxCd1â^'xO alloys. Superlattices and Microstructures, 2007, 42, 165-171.	1.4	24
52	The spin effect in zinc-blende and diluted magnetic semiconductors: FP-LAPW study. Physica B: Condensed Matter, 2010, 405, 625-631.	1.3	22
53	Half-Metallic Ferromagnetism in Double Perovskite Ca₂CoMoO₆ Compound: DFT+U Calculations. Spin, 2017, 07, 1750009.	0.6	22
54	First-principles study of cubic AlxGa1â^'xN alloys. Computational Materials Science, 2005, 33, 136-140.	1.4	21

#	Article	IF	Citations
55	Structure and magnetic properties of the 3d transition-metal mono-borides TMâ€“B (TM=Mn, Fe, Co) under pressures. Journal of Magnetism and Magnetic Materials, 2014, 365, 23-30.	1.0	21
56	Energy band structure calculation of GexSn1â^'x and SixSn1â^'x alloys. Infrared Physics and Technology, 1995, 36, 967-972.	1.3	20
57	Meta-GGA calculation of the electronic structure of group IIIâ€“V nitrides. Physica Status Solidi (B): Basic Research, 2006, 243, 1577-1582.	0.7	20
58	Structural and electronic properties calculations of BexZn1â^'xSe alloy. Materials Science in Semiconductor Processing, 2007, 10, 6-13.	1.9	20
59	First-principles calculations of the structural, electronic and optical properties of cubic BxGa1â^'xAs alloys. Physica B: Condensed Matter, 2012, 407, 1292-1300.	1.3	20
60	First-principles investigation on structural, elastic, electronic and thermodynamic properties of filled skutterudite PrFe₄P₁₂compound for thermoelectric applications. Molecular Simulation, 2014, 40, 1236-1243.	0.9	20
61	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.	0.8	20
62	A theoretical investigation of ZnOxS1â€“x alloy band structure. Physica Status Solidi (B): Basic Research, 2007, 244, 1560-1566.	0.7	19
63	Electronic properties and stability of ZnO from computational study. Physica B: Condensed Matter, 2008, 403, 3154-3158.	1.3	19
64	ELECTRONIC AND OPTICAL PROPERTIES OF BaO, BaS, BaSe, BaTe AND BaPo COMPOUNDS UNDER HYDROSTATIC PRESSURE. Modern Physics Letters B, 2009, 23, 3065-3079.	1.0	19
65	First-Principles Calculations of Structural, Electronic, Optical, and Thermodynamic Properties of CdS, CdTe and Their Ternary Alloys CdS_{1-x}Te_x(0.0 â‰¤ x â‰¤1.0). Acta Physica Polonica A, 2014, 125, 1110-1117.	0.2	19
66	Rattling Heusler semiconductors' thermoelectric properties: First-principles prediction. Chinese Journal of Physics, 2019, 57, 195-210.	2.0	19
67	Electronic structure of AlxGa1 â^' xAs and GaPxAs1 â^' 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.	1.7	18
68	First-principle study of structural, elastic and electronic properties of Th monopnictides. Journal of Nuclear Materials, 2014, 454, 186-191.	1.3	18
69	Electronic and Optical Properties of Copper Halide Mixed Crystals CuBr1?xIx. Physica Status Solidi (B): Basic Research, 1998, 209, 339-352.	0.7	17
70	First principles calculations of structural, electronic and optical properties of BAs1â^'xPx alloy. Physics Procedia, 2009, 2, 933-940.	1.2	17
71	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.	1.3	17
72	Empirical Pseudo-Potential Calculations in GaAs1?xNx and AlAs1?xNx Ordered Alloys. Physica Status Solidi (B): Basic Research, 1997, 201, 117-134.	0.7	16

#	Article	IF	Citations
73	Theoretical investigation of electronic structure of PbSxTe1â^'x and PbSexTe1â^'x alloys. Materials Chemistry and Physics, 2009, 114, 650-655.	2.0	16
74	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.	1.3	16
75	Electronic structure and magnetism of cubic Ga1â^'xEuxN and Al1â^'xEuxN using the LSDA+U approach. Computational Materials Science, 2010, 48, 743-748.	1.4	16
76	Half-metallic ferromagnetism in ZnCrTe and CdCrTe: Ab initio study. Computational Materials Science, 2011, 50, 2785-2792.	1.4	16
77	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.	1.9	16
78	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.	2.0	16
79	Theoretical analysis of disorder effects on electronic and optical properties in InGaAsP quaternary alloy. Journal of Applied Physics, 1997, 82, 4923-4930.	1.1	15
80	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.	1.4	15
81	Investigated electronic structure and magnetic ordering of rare earth impurities (Eu, Gd) in ZnO. International Journal of Modern Physics B, 2016, 30, 1650225.	1.0	15
82	Structural, electronic and optical properties of cubic fluoroelpasolite Cs2NaYF6 by density functional theory. Chinese Journal of Physics, 2018, 56, 1756-1763.	2.0	15
83	Ab initio study of cubic PbSxSe1â^'x alloys. Journal of Alloys and Compounds, 2008, 462, 135-141.	2.8	14
84	Ab initio studies of structural, elastic and electronic properties of ZrxNb1â^'xC and ZrxNb1â^'xN alloys. Physica B: Condensed Matter, 2010, 405, 153-157.	1.3	14
85	Half-Metallic and Half-Semiconductor Gaps in Cr-Based Chalcogenides: DFT + U Calculations. Journal of Superconductivity and Novel Magnetism, 2019, 32, 635-649.	0.8	14
86	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.	0.9	14
87	The electronic structure of CuCl. Computational Materials Science, 2001, 20, 267-274.	1.4	13
88	Theoretical analysis of disorder effects on electronic and optical properties of the quaternary alloy In1â€“xGaxAsySb1â€“y epilayer on GaSb and InAs. Physica Status Solidi (B): Basic Research, 2003, 238, 156-172.	0.7	13
89	First-principle calculations of electronic and positronic properties of AlGaAs2. Physica B: Condensed Matter, 2007, 396, 169-176.	1.3	13
90	First principle calculations of structural, electronic and thermodynamic properties of Al3(TixV1â^'x) alloy in D022 and L12 structures. Solid State Sciences, 2013, 16, 1-5.	1.5	13

#	Article	IF	Citations
91	Half metallic properties of the quaternary CuFe2GaSe4 chalcogenide compound. Computational Materials Science, 2014, 85, 159-163.	1.4	13
92	Electronic and optical properties of copper halides mixed crystal CuCl1 â˜' xBrx. Journal of Physics and Chemistry of Solids, 1998, 59, 997-1007.	1.9	12
93	Interband transitions of wide-band-gap ternary pnictide BeCN2 in the chalcopyrite structure. Physica Status Solidi (B): Basic Research, 2004, 241, 305-316.	0.7	12
94	First principles calculations of structural, electronic, thermodynamic and optical properties of BAs_{1 -x}P_xalloy. Physica Scripta, 2009, 79, 045002.	1.2	12
95	Thermodynamic, structural and electronic, properties of SnO2: By GGA and GGA + trans-blaha-modified Beckeâ€"Johnson (TB-mBJ) calculation. Superlattices and Microstructures, 2015, 84, 80-90.	1.4	12
96	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.	0.8	12
97	First-principles study of the electronic structure, magnetism, and phonon dispersions for CaX (XÂ= C,) Tj ETQq1 1 0.784314 rgBT /Ov	0.9	12
98	Ferromagnetism in RaBi with Zinc-Blende and Wurtzite Structures: Ab-initio Prediction. Spin, 2018, 08, 1850008.	0.6	12
99	First-Principles Study of Ferromagnetism in Iron Chromite Spinels: FeCr₂O₄ and CrFe₂O₄. Spin, 2019, 09, .	0.6	12
100	Band structure calculations of Ga1 â˜' xAlxAs, GaAs1 â˜' xPx and AlAs under pressure. Computational Materials Science, 1995, 3, 393-401.	1.4	11
101	Vacancy effects on structural and electronic properties of 4d transition-metal carbides. Computational Materials Science, 2009, 44, 1071-1075.	1.4	11
102	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.	1.0	11
103	Spin-Polarized Calculations of Magnetic and Thermodynamic Properties of the Full-Heusler $$mathrm{{Co}}_{2}$$ Co 2 MnZ (ZÂ=ÂAl, Ga). International Journal of Thermophysics, 2013, 34, 507-520.	1.0	11
104	A datamining approach to predict the formation enthalpy for rare-earth dihydrides REH2 (REÂ=ÂCe,Pr,Dy). International Journal of Hydrogen Energy, 2016, 41, 11254-11263.	3.8	11
105	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.	0.8	11
106	Sn₃C₂ monolayer with transition metal adatom for gas sensing: a density functional theory studies. Nanotechnology, 2021, 32, 355502.	1.3	11
107	First-principles study of electronic structure and magnetism of cubic Al1â˜'xErxN using the LSDA+U approach. Journal of Magnetism and Magnetic Materials, 2011, 323, 1174-1178.	1.0	10
108	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.	0.8	10

#	Article	IF	Citations
109	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.	1.0	10
110	Ab-Initio Prediction of Intrinsic Half-Metallicity in Binary Alkaliâ€“Metal Chalcogenides: KX (X=S, Se and) Tj ETQq0 0 0 rgBT /Overlock 10	0.6	10
111	DFT + U studies of the electronic and optical properties of ReS₂ mono-layer doped with lanthanide atoms. Materials Research Express, 2019, 6, 106307.	0.8	10
112	Electronic structure and optical properties of (ZnSe)nâ•(Si2)m (111) superlattices. Journal of Applied Physics, 2006, 99, 043702.	1.1	9
113	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.	1.9	9
114	Structural and elastic properties of TiN and AlN compounds: first-principles study. Materials Science-Poland, 2014, 32, 220-227.	0.4	9
115	Realization of p-Type Conductivity in ZnO via Potassium Doping. Acta Physica Polonica A, 2016, 129, 1155-1158.	0.2	9
116	Calculation of the electronic and elastic properties of carbon. Journal of Physics Condensed Matter, 1998, 10, 3195-3200.	0.7	8
117	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.	0.8	8
118	Electronic structure of cubic ErxGa1â˜'xN using the LSDA+U approach. Physica B: Condensed Matter, 2008, 403, 2702-2706.	1.3	8
119	The spin effect in zinc-blende CdEuS and CdEuSe: GGA and GGA+U studies. Physica B: Condensed Matter, 2012, 407, 3639-3645.	1.3	8
120	FP-LMTO method to calculate the structural, thermodynamic and optoelectronic properties of Si_xGe_{1â˜'}_xC alloys. Molecular Physics, 2013, 111, 3208-3217.	0.8	8
121	Ferromagnetism in CdOX (X=Mn and N) with and without intrinsic point defects: A density functional theory. Results in Physics, 2013, 3, 205-208.	2.0	8
122	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.	1.0	8
123	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.	0.8	8
124	First-Principles Studies of Structural, Electronic and Magnetic Properties of the CrS, CrSe and CrTe Compounds. Spin, 2018, 08, 1850019.	0.6	8
125	Thermoelectric and Half-Metallic Behavior of the Novel Heusler Alloy RbCrC: Ab initio DFT Study. Spin, 2020, 10, .	0.6	8
126	Ordering effects on the electronic structures of AlN/GaN, InN/GaN and InN/AlN superlattices. Computational Materials Science, 2005, 33, 157-162.	1.4	7

#	Article	IF	Citations
127	Electronic structure and magnetic ordering in gadolinium-doped AlGaN from LSDA + U calculations. International Journal of Computational Materials Science and Engineering, 2018, 07, 1850019.	0.5	7
128	Density functional theory studies of the SrC and SrN compounds. Materials Chemistry and Physics, 2019, 237, 121875.	2.0	7
129	First-Principles Study of the New Half-Metallic Ferromagnetic Quaternary-Heusler Alloys NaXNO (X=Ca, Sr, Ba). Spin, 2020, 10, .	0.6	7
130	Ab-initio investigation of optoelectronic properties for elpasolite Cs2NaVCl6 using GGA+U approach: Band gap engineering. Computational Condensed Matter, 2021, 26, e00531.	0.9	7
131	The large rotations theory of elastoâ€viscoplastic shells subjected to the dynamic and thermal loads. Engineering Computations, 2003, 20, 366-389.	0.7	6
132	Correlation effects on the electronic structure of Co2Mn0.5Fe0.5Si and Co2Mn0.5Gd0.5Si quaternary alloys. Intermetallics, 2013, 37, 27-31.	1.8	6
133	First-principles calculations of magnetic properties for CdCrO2 under pressure. Journal of Magnetism and Magnetic Materials, 2013, 327, 76-78.	1.0	6
134	Electronic and magnetic properties of Fe2SiC. European Physical Journal B, 2014, 87, 1.	0.6	6
135	Structural Stability, Electronic and Magnetic Properties of (Ni1â^'xCox)2MnSn Quaternary Heusler Alloys. Spin, 2017, 07, 1750010.	0.6	6
136	Pressure dependence of electronic properties in zinc-blende-like SiGe compound. Journal of Physics and Chemistry of Solids, 1998, 59, 759-768.	1.9	5
137	Theoretical analysis of disorder effects on electronic and optical properties of the quaternary alloy Ga1â^'xAlxAsySb1â^'y. Materials Chemistry and Physics, 2002, 74, 328-335.	2.0	5
138	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.	1.0	5
139	Predicted modifications in the direct and indirect gaps of Si. Solid State Communications, 1995, 96, 245-250.	0.9	4
140	Tight-Binding Calculation of Electronic and Elastic Properties of Ge. Physica Status Solidi (B): Basic Research, 2000, 217, 911-917.	0.7	4
141	Predictive study of electronic properties of siliconâ€"carbon alloys. Materials Science and Engineering B: Solid-State Materials for Advanced Technology, 2005, 122, 145-151.	1.7	4
142	Structural, electronic and energetic properties of silicon carbon alloys. Physica B: Condensed Matter, 2007, 388, 167-173.	1.3	4
143	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.	1.3	4
144	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.	0.5	4

#	Article	IF	Citations
145	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.	0.9	4
146	Predicted dynamically stable new phase for CrO2 compound: DFTÂ+ U calculations. Computational Condensed Matter, 2019, 21, e00400.	0.9	4
147	Electronic Structure and Thermoelectric Properties of Semiconductors K₂GeSiX₆ (X=F, Cl, Br and I) Compounds: Ab-Initio Investigation. Spin, 2021, 11, .	0.6	4
148	DFT studies on the structural, electronic, and optical properties of Na2ZnP2O7 compound. Materials Today Communications, 2021, 29, 102868.	0.9	4
149	Prediction of High Pressure Phase Transition in Al Compounds by the Ionicity Character. Physica Status Solidi (B): Basic Research, 1995, 189, K5.	0.7	3
150	Transferable Non-Orthogonal Tight-Binding Model for Silicon. Physica Status Solidi (B): Basic Research, 1998, 208, 413-426.	0.7	3
151	First-Principles Calculation of Structural and Electronic Properties of Wurtzite AlxGa1â€”xN, InxGa1â€”xN, and InxAl1â€”xN Random Alloys. Physica Status Solidi C: Current Topics in Solid State Physics, 2003, 0, 315-319.	0.8	3
152	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.	1.3	3
153	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.	1.3	3
154	A Computational Study of the Electronic and Magnetic Properties of Rare Earth (Er)-Doped InGaN. Spin, 2018, 08, 1850011.	0.6	3
155	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.	0.9	3
156	Prediction of a Dynamically Stable New Half-Metallic Phase for the BaN and BaC Compounds. Journal of Superconductivity and Novel Magnetism, 2019, 32, 2031-2044.	0.8	3
157	Competition between the hcp nonmagnetic and antiferromagnetic phases in the transition path of Fe under pressure. Journal of Magnetism and Magnetic Materials, 2020, 499, 166312.	1.0	3
158	Ab initio studies of the structural, electronic and magnetic properties of stannite CuFe2-III-VI4 (IIIÂ= Al,) Tj ETQq0 0 0 rgBT /Overlock 10	0.9	3
159	Electronic structure, mechanical and thermoelectric properties of the full Heusler Ba2AgZ (Zâ€‰=â€‰Bi, Sb) alloys: insights from DFT study. Indian Journal of Physics, 2021, 95, 2675-2686.	0.9	3
160	Positron Energy Levels in Cd-Based Semiconductors. Communications in Theoretical Physics, 2013, 59, 756-762.	1.1	2
161	Resonant Electromagnetic Field Distribution on Doped Multilayer Thin Film Structure. Spectroscopy Letters, 2014, 47, 397-403.	0.5	2
162	First-principles prediction of insulating antiferromagnet in ordered double-perovskite Ca2MnMoO6 compound. International Journal of Computational Materials Science and Engineering, 2017, 06, 1750027.	0.5	2

#	Article	IF	Citations
163	Prediction of Half-Metallic Properties in Non-transition Metal-based Binary Compounds X Bi (X = Ba, Sr) Tj ETQq1 1 0.784314 rgBT /Over Magnetism, 2018, 31, 2767-2776.	0.8	2
164	First principles predictions of electronic and elastic properties of BaPb 2 As 2 in the ThCr 2 Si 2 -type structure. Physica C: Superconductivity and Its Applications, 2018, 544, 18-21.	0.6	2
165	First-Principle Studies of Ferrimagnetic Double Perovskite Ca2FeMoO6 Compound. Journal of Superconductivity and Novel Magnetism, 2019, 32, 2913-2922.	0.8	2
166	Spin-polarized optical properties of half-metallic binary XBi (Xâ€‰=â€‰Ca, Sr and Ba) compounds in zinc blende and wurtzite phases. Indian Journal of Physics, 2019, 93, 627-638.	0.9	2
167	Theoretical study of structural, electronic, dynamic and thermodynamic properties of Ni2FeAl and Ni2CoAl alloys. Computational Condensed Matter, 2020, 24, e00480.	0.9	2
168	Full-potential electronic structure calculations of InN(AlN) layer embedded in GaN bulk. Physica Status Solidi (A) Applications and Materials Science, 2006, 203, 2247-2253.	0.8	1
169	Electronic structure of new RENiAsO (RE = Rare Earth Elements) compounds: Ab initio spin-density functional theory. Superlattices and Microstructures, 2009, 46, 533-540.	1.4	1
170	Positron energy levels in zinc chalcogenides ZnS, ZnSe, and ZnTe. Computational Materials Science, 2014, 93, 22-28.	1.4	1
171	First-Principles Calculations of the Structure and Magnetic Phases of FeAs2 Compound under Pressure. Spin, 2018, 08, 1850016.	0.6	1
172	A first-principles study of the structural, elastic, electronic, vibrational, and optical properties of BaSe1â^'xTex. Journal of Computational Electronics, 2018, 17, 1478-1491.	1.3	1
173	An ab initio study on the transition path of carbon dioxide at high pressure: Evidence for a new intermediate P4â€¾m2 phase. Computational Condensed Matter, 2019, 21, e00429.	0.9	1
174	Electronic structure theory of unusually matched BAs1-xPx alloys using high-throughput ab-initio computation. Physica B: Condensed Matter, 2020, 579, 411901.	1.3	1
175	Effect of an interfacial oxygen monolayer on the spin-polarization at the Fe/MgO interface: First-principles calculations. Materials Science in Semiconductor Processing, 2021, 121, 105463.	1.9	1
176	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.	0.7	1
177	Predicted modifications in the direct and indirect gaps of GaP. Infrared Physics and Technology, 1995, 36, 791-797.	1.3	0
178	Effect of Pressure on the energy band gaps of InxGa1-xN and InxAl1-xN. Materials Research Society Symposia Proceedings, 2002, 743, L11.25.1.	0.1	0
179	First-principles calculations of the structural and electronic properties of the III-nitrides-based superlattices. Physica E: Low-Dimensional Systems and Nanostructures, 2003, 17, 235-237.	1.3	0
180	Strong dependence of the fundamental band gap on the alloy composition in cubic InxGa1-xN and InxAl1-xN alloys. Materials Research Society Symposia Proceedings, 2003, 798, 640.	0.1	0

#	Article	IF	Citations
181	Theoretical studies of the angular correlation of positron annihilation in Al1â˜' x In x N. Physica Status Solidi (B): Basic Research, 2004, 241, 876-884.	0.7	0
182	Contribution to the study of electronic structure of crystalline semiconductors (Si, Ge, GaAs, Gap,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50	0.1	0
183	Geometry of Waves Guides for Containment of Propagating Resonant Modes. Journal of Fundamental and Applied Sciences, 2015, 3, 68.	0.2	0
184	Magnetic ordering and electronic structure of the ternary iron arsenide BaFe2As2. International Journal of Modern Physics B, 2015, 29, 1550182.	1.0	0
185	Fermi Surfaces of Compensated and Uncompensated Metals: GGA+U+SO Comparative Ab Initio Study. Journal of Superconductivity and Novel Magnetism, 2016, 29, 2195-2201.	0.8	0