First-principles calculations to investigate structural ar Ni2LaZ (Zâ€**%â**€**%s**, Sb and Bi) Heusler alloys

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Citation Report

#	Article	IF	CITATIONS
1	Firstâ€principles calculations to investigate structural stabilities, mechanical and optoelectronic properties of <scp>NbCoSn</scp> and <scp>NbFeSb halfâ€Heusler</scp> compounds. International Journal of Quantum Chemistry, 2021, 121, e26582.	2.0	32
2	Pressure dependence of structural, elastic, electronic, thermodynamic, and optical properties of van der Waals-type NaSn2P2 pnictide superconductor: Insights from DFT study. Results in Physics, 2021, 21, 103848.	4.1	48
3	Electronic structure, elastic, optical and thermodynamic properties of cubic perovskite NaBaF3 with pressure effects: First-principles calculations. Results in Physics, 2021, 22, 103860.	4.1	28
4	The Ferromagnetism Stability Induced by (Ti, V, and Cr)-Doped LiMgN Alloy for the Spintronic Application: First-Principle Calculations. Journal of Superconductivity and Novel Magnetism, 2021, 34, 1915-1921.	1.8	5
5	First-principles calculations to investigate mechanical, optoelectronic and thermoelectric properties of half-Heusler p-type semiconductor BaAgP. Results in Physics, 2021, 23, 104068.	4.1	25
6	Investigation of the stability, electronic structure, and magnetic properties of Sc2VZ (ZÂ=ÂGe, Si) Heusler alloys: First-principles calculations. Materials Science and Engineering B: Solid-State Materials for Advanced Technology, 2021, 267, 115096.	3.5	2
7	First-principles calculations of adsorption sensitivity of Au-doped MoS2 gas sensor to main characteristic gases in oil. Journal of Materials Science, 2021, 56, 13673-13683.	3.7	27
8	Theoretical investigation on the structural, mechanical, electronic and thermodynamic properties of cubic Ti3NiAl2C compound. Physica B: Condensed Matter, 2021, 609, 412917.	2.7	0
9	Structural, Elastic, Electronic, and Magnetic Properties of XPtBi (X=Er and Ho) Using FP-LAPW Method. Journal of Superconductivity and Novel Magnetism, 2021, 34, 1865-1873.	1.8	3
10	Investigation of the thermoelectric properties of Lithium-Aluminium-Silicide (LiAlSi) compound from first-principles calculations. Computational Condensed Matter, 2021, 27, e00551.	2.1	10
11	The crystal and electronic structures, dynamical stabilities and thermal properties, elastic constants and mechanical stabilities, Born effective charges and dielectric constants of a novel tetragonal ZrO2 phase: First-principles calculations. Journal of Physics and Chemistry of Solids, 2021, 154, 110046.	4.0	9
12	First-principles calculations to investigate the electronic and optical properties of (MoS2)4-n/(MoSSe)n lateral heterostructure. Journal of Physics and Chemistry of Solids, 2021, 154, 110049.	4.0	8
13	First-principles calculations to investigate structural, electronic and optical properties of Na based fluoroperovskites NaXF3 (X= Sr, Zn). Solid State Communications, 2021, 334-335, 114396.	1.9	12
14	Stability and mechanical, electronic, and optical investigations of a new Heusler alloy: Ag2ScGe. Results in Physics, 2021, 27, 104518.	4.1	3
15	First-principles calculations to investigate pressure effect on mechanical and thermal properties of ZrAl2. Computational and Theoretical Chemistry, 2021, 1202, 113304.	2.5	2
16	First-principles calculations to investigate electronic structure and magnetic, mechanical and thermodynamic properties of d0 half-Heusler LiXN (X= Na, K, Rb) alloys. Solid State Sciences, 2021, 118, 106633.	3.2	11
17	Sulfur doping effect on the electronic properties of zirconium dioxide ZrO2. Materials Science and Engineering B: Solid-State Materials for Advanced Technology, 2021, 270, 115200.	3.5	28
18	Adsorption, sensing and optical properties of molecules on BC3 monolayer: First-principles calculations. Materials Science and Engineering B: Solid-State Materials for Advanced Technology,	3.5	16

#	Article	IF	CITATIONS
19	First-principles calculations to investigate half-metallic band gap and elastic stability of Co(Mo,Tc)MnSb compounds. Physica E: Low-Dimensional Systems and Nanostructures, 2021, 133, 114790.	2.7	12
20	Structural, elastic, electronic, thermal, and phononic properties of yttrium carbide: First-principles calculations. Materials Chemistry and Physics, 2021, 270, 124744.	4.0	9
21	First-principles calculations to investigate stability, electronic and optical properties of fluorinated MoSi2N4 monolayer. Results in Physics, 2021, 30, 104864.	4.1	19
22	First-principles calculations to investigate structural, elastic, electronic, lattice dynamic and optical properties for scandium and yttrium nitrides in zinc blend structure. Journal of Materials Research and Technology, 2021, 14, 1958-1968.	5.8	6
23	First-principles calculations to investigate electronic structure and transport properties of CrC monolayers: A new horizon for spintronic application. Materials Science and Engineering B: Solid-State Materials for Advanced Technology, 2021, 272, 115379.	3.5	17
24	Investigation of the structural, electronic, magnetic, and optical properties of CsXO3 (X = Ge, Sn, Pb) perovskites: A first-principles calculations. Optik, 2021, 244, 167536.	2.9	21
25	First-principles calculations to investigate structural, magnetic, electronic and elastic properties of full-Heusler alloys Co2MB (M=V, Mn). Solid State Communications, 2021, 337, 114426.	1.9	4
26	A new method for calculating the thermodynamic and physical properties of compounds: Application to Laves phase Fe2Mo. Physica B: Condensed Matter, 2021, 621, 413307.	2.7	4
27	First-principles calculations to investigate electronic, optical, thermodynamic and thermoelectric properties of new Na6ZnX4 (X=O, S, Se) ternary alloys. Journal of Physics and Chemistry of Solids, 2022, 160, 110305.	4.0	18
28	Designing a sp3 structure of carbon T-C9: First-principles calculations. Results in Physics, 2020, 19, 103690.	4.1	16
29	First-principles calculation to investigate the influence of shear deformation on the electronic structure and optical properties of hydrogenated silicene. Computational and Theoretical Chemistry, 2022, 1207, 113506.	2.5	0
30	First-principles calculations to investigate structural, mechanical, electronic, magnetic and thermoelectric properties of Ba2CaMO6 (M=Re, Os) cubic double perovskites. Physica B: Condensed Matter, 2022, 626, 413554.	2.7	8
31	First-principles calculations to investigate electronic structures, ferromagnetic and optical properties of SnSe2 doped with double impurities. Materials Chemistry and Physics, 2022, 277, 125459.	4.0	1
32	First-principles calculations of optical properties of 2D CaFBr and BaFBr monolayers. Physica E: Low-Dimensional Systems and Nanostructures, 2022, 137, 115074.	2.7	13
33	Electronic, magnetic and elastic calculations on half-metallic Heusler Ti ₂ RuTl compound. Philosophical Magazine, 2022, 102, 153-165.	1.6	1
34	First-principles calculations to investigate electronic structure and optical properties of 2D MgCl2 monolayer. Superlattices and Microstructures, 2022, 162, 107132.	3.1	15
35	First principal calculations to investigate structural, electronic, optical, and magnetic properties of Fe3O4and Cd-doped Fe2O4. Computational Condensed Matter, 2022, 30, e00629.	2.1	15
36	First-principles calculations to investigate electronic, magnetism, elastic properties of TbxDy1-xFe2 (xÂ=Â0, 0.25, 0.5, 1). Journal of Magnetism and Magnetic Materials, 2022, 547, 168953.	2.3	4

#	Article	IF	CITATIONS
37	First-principles calculations to investigate stability, electronic properties and anisotropy of half-metallic full Heusler alloy Co2NbGa. Results in Physics, 2022, 34, 105237.	4.1	8
38	First-principles calculations to investigate structural, electronics, optical and elastic properties of Sn-based inorganic Halide-perovskites CsSnX3 (XÂ=Âl, Br, Cl) for solar cell applications. Computational and Theoretical Chemistry, 2022, 1209, 113624.	2.5	42
39	First-principles calculations to investigate variation of cationic-ligand LmAl2Ge2 (Lm = Ca, Y, La and Ce). Indian Journal of Physics, 2022, 96, 3151-3159.	1.8	5
40	First-principles quantum analysis on the role of V-doping on the tuning of electronic and optical properties of spinel oxides MnTi2O4. Materials Science and Engineering B: Solid-State Materials for Advanced Technology, 2022, 278, 115643.	3.5	10
41	First-principles calculations to investigate transformation of optically inactive zinc-blend beryllium chalcogenides to optically active semiconductor alloys through doping of Hg atom(s). Physica B: Condensed Matter, 2022, , 413881.	2.7	1
42	First-principles study of structural, mechanical, lattice dynamics, superconducting and optoelectronic properties of the Pd3Pb2Se2 shandite under hydrostatic pressure. Physica B: Condensed Matter, 2022, , 413920.	2.7	3
43	First-principles calculations to investigate elastic and thermodynamic properties of FeAlNixCrMn quinternary alloys. Journal of Materials Research and Technology, 2022, 18, 1322-1332.	5.8	7
44	First-principles calculations to investigate Structural, electronic, and optical properties of MgF2 monolayer in 1T-phase and 2H-phase using hybrid functional. Chemical Physics, 2022, 557, 111473.	1.9	1
45	First-principles calculations to investigate the interfacial energy and electronic properties of Mg/AlN interface. Journal of Physics and Chemistry of Solids, 2022, 167, 110705.	4.0	15
46	First-principles calculations to investigate elasto-mechanical and opto-electronic properties of pyrochlore oxides X2Zr2O7 (X=La, Nd). Journal of Materials Research and Technology, 2022, 18, 5005-5018.	5.8	3
47	First-principles calculations to investigate influence of transition metals TM (TMÂ=ÂTi, Zr, Hf) on elastic properties and thermodynamic properties of ScB12 and YB12 dodecaborides. Chemical Physics Letters, 2022, 800, 139680.	2.6	9
48	First-principles calculations to investigate structural, electronic and phonon properties of sodium bromide (NaBr) and sodium iodide (NaI) crystals. Computational Condensed Matter, 2022, 31, e00682.	2.1	1
49	First-principles calculations to investigate transport properties of non-trivial fermions of CoSi. Computational Condensed Matter, 2022, 31, e00686.	2.1	1
50	First-principles calculations to investigate structural, elastic, electronic and optical properties of A2OsH6 for storage hydrogen and optoelectronic devices. Computational Condensed Matter, 2022, 31, e00684.	2.1	3
51	First-principles calculations to investigate strain-tunable electronic bandgap of black phosphorus-structured nitrogen with desirable optical and elastic properties. Materials Science and Engineering B: Solid-State Materials for Advanced Technology, 2022, 281, 115745.	3.5	3
52	First-principles calculations to investigate structural, electrical, and optical properties of half Heusler alloy LiCrN. Physics Letters, Section A: General, Atomic and Solid State Physics, 2022, 442, 128178.	2.1	3
53	First-principles calculations to investigate static and dynamic stability, electronic, optical and thermoelectric of Zr2TiSi Heuslerene. Chemical Physics, 2022, 560, 111585.	1.9	2
54	First-Principles Calculations to Investigate Structural, Electronic, Optical, and Elastic Properties of Ceria. Advances in Condensed Matter Physics, 2022, 2022, 1-11.	1.1	0

#	Article	IF	CITATIONS
55	First-principles calculations to investigate variation in the bandgap of NaSrF3 Fluoro-Perovskite with external static isotropic pressure and its Impact on optical properties. Computational and Theoretical Chemistry, 2022, 1214, 113766.	2.5	21
56	First-principles calculations to investigate structural phase transformation to semi-conductor–metal transition and their impact on optical properties in lead titanium oxynitrate. Molecular Simulation, 0, , 1-9.	2.0	1
57	Computational Study of the Structural, Mechanical, Electronic, Half-Metallic, and Magnetic Properties of CoCrYZ (Z = In, Sn, Tl, and Pb) Quaternary Heusler Alloys. Journal of Superconductivity and Novel Magnetism, 2022, 35, 2837-2850.	1.8	4
58	First-principles calculations to investigate new ferromagnetic quaternary Heusler alloys FeZrTiZ(Z=Si, Sn, Pb): Compatible for spin polarized device and waste heat recovery applications. Solid State Sciences, 2022, 132, 106964.	3.2	4
59	First-principles calculations to investigate band gap of cubic BaThO3 with systematic isotropic external static pressure and its impact on structural, elastic, mechanical, anisotropic, electronic and optical properties. Journal of Physics and Chemistry of Solids, 2022, 169, 110878. Hexagonal,	4.0	14
60	Inclinic, and Monoclinic Structures of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si22.svg" display="inline" id="d1e768"><mml:mi>α</mml:mi>-BiFeO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si23.svg" display="inline"</mml:math </mml:math 	3.5	4
61	Ab-Initio Study of Structural, Mechanical, and Dynamical Stability, Electronic, Thermal, and Optical Properties of Silver Halide Agx (X = F, Cl, Br, and I) Semiconductors. SSRN Electronic Journal, O, , .	0.4	0
62	First-principles calculations to investigate elastic properties, ideal tensile strength and electronic properties of TiSi, Ti5Si3 and Ti5Si4. Chemical Physics Letters, 2022, 806, 139992.	2.6	2
63	First-principles Calculations to Investigate Emerging Double Perovskites K2NaMoX6 (X=Cl, I) Compounds for Magnetic and Optoelectronic Applications. Physica B: Condensed Matter, 2022, 645, 414252.	2.7	5
64	First-principles investigation of effects of defects on the physical properties of 3C-SiC under high temperatures and pressures. Journal of Materials Research and Technology, 2022, 20, 3633-3645.	5.8	3
65	First-principles calculations to investigate strain effects on structural, electronic, elastic and transport properties of Cs2PdBr6. Computational and Theoretical Chemistry, 2022, 1215, 113833.	2.5	8
66	First-principles calculations to investigate strong half-metallic ferromagnetic and thermoelectric sensibility of LiCrX (XÂ=ÂS, Se, and Te) alloys. Journal of Magnetism and Magnetic Materials, 2022, 562, 169822.	2.3	10
67	First-principles calculations to investigate structural, electronic, mechanical, optical, thermophysical and vibrational properties of TaFeSb. International Journal of Modern Physics B, 2022, 36, .	2.0	2
68	Optical and electronic properties of defect chalcopyrite ZnGa2Se4: Experimental and theoretical investigations. Solid State Communications, 2022, 356, 114950.	1.9	19
69	First-principles calculations to investigate structural, electronic and optical properties of two-dimensional ZnIn2S4. Applied Surface Science, 2022, 605, 154739.	6.1	2
70	First-principles calculations to investigate structural, electronics, optical and mechanical properties of LaRu ₂ P ₂ compound for superconducting application. Molecular Simulation, 2023, 49, 76-84.	2.0	6
71	First-Principle Calculations to Investigate Structural, Electronic, Elastic, Mechanical, and Optical Properties of K2CuX (X=As, Sb) Ternary Compounds. Advances in Materials Science and Engineering, 2022, 2022, 1-10.	1.8	5
72	First-principles calculations to investigate structural, dynamical, thermodynamic and thermoelectric properties of CdYF3 perovskite. Computational and Theoretical Chemistry, 2022, 1217, 113928.	2.5	18

#	Article	IF	CITATIONS
73	First-principles calculations to investigate structural, elastic, optical, and thermoelectric properties of narrow band gap semiconducting cubic ternary fluoroperovskites barium based BaMF3 (M = Ag and) Tj ETQ	q0 0 :ᡚ 8gBT	/O v erlock 10
74	xmins:mml="http://www.w3.org/1998/Math/MathML" altimg="si62.svg" display="inline" id="d1e591"> <mml:msub> <mml:mrow /> <mml:mrow> <mml:mn> 4</mml:mn></mml:mrow> </mml:mrow </mml:msub> GaPbX <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si63.svg" display="inline"</mml:math 	1.9	7
75	Study of electronic, structural and magnetic properties of electrodeposited Co2MnSn Heusler alloy thin films. Journal of Materials Research and Technology, 2023, 22, 1-16.	5.8	5
76	First-principles calculations to investigate structural, electronic, optical, and magnetic properties of a scintillating double perovskite halide (Cs2LiCeCl6). Journal of Materials Research and Technology, 2022, 21, 4790-4798.	5.8	19
77	First-principles calculations to investigate structural stability, half-metallic behavior, thermophysical and thermoelectric properties of Co2YAl (YÂ=ÂMo, Tc) full Heusler compounds. Computational and Theoretical Chemistry, 2023, 1219, 113943.	2.5	17
78	First-principles calculations to investigate HgY2S/Se4 spinel chalcogenides for optoelectronic and thermoelectric applications. Journal of Materials Research and Technology, 2023, 22, 97-106.	5.8	5
79	First-principles calculations to investigate magnetic, electronic, mechanical and dynamical properties of the bimetallic M-Pt (M: Mn Co and Ni) alloys. Journal of Magnetism and Magnetic Materials, 2023, 565, 170298.	2.3	2
80	First-principles calculations to investigate structural, electronic, optical, thermoelectric, magnetic, and magnetocaloric properties of the orthochromite EuCrO3. Computational and Theoretical Chemistry, 2023, 1220, 113993.	2.5	4
81	First-principles calculations to investigate third-order elastic constant, anharmonicity and temperature dependent second elastic constant of thermoelectric materials Cu3MSe4(MÂ=ÂV and Nb). Chemical Physics Letters, 2023, 812, 140254.	2.6	1
82	First-principles calculations to investigate physical properties of three magnetic sub lattice CaCu3Mn4-xlrxO12 (x = 0, 2 and 4) system via symmetry evaluation. Materials Chemistry and Physics, 2023, 295, 127164.	4.0	6
83	First-principles calculations to investigate structural, elastic, electronic and thermoelectric properties of narrow-band gap half-Heusler RhV <i>X</i> (<i>X</i> = Si, Ge) compounds. International Journal of Modern Physics B, 2023, 37, .	2.0	3
84	First-principles calculations to investigate structural, elastic, electronic and thermodynamic properties of NbCoSn and VRhSn Half-Heusler compounds. Results in Physics, 2022, 43, 106132.	4.1	5
85	First principles computation of insulator–semiconductor–metal transition and its impact on structural, elastic, mechanical, anisotropic and optical properties of CsSrF ₃ under systematic static isotropic pressure. Molecular Simulation, 2023, 49, 453-471.	2.0	2
86	First-principles calculations to investigate structural, elastic, electronic, optical, and magnetic properties of Hg2WO4 for photocatalytic applications. Optik, 2023, 274, 170565.	2.9	1
87	First-principles calculations for comparative band structure study of SrTiO3 perovskite on bulk and layered phases for efficient optoelectronic conversion. Computational and Theoretical Chemistry, 2023, 1220, 114006.	2.5	4
88	Band gap tuning of non-toxic Sr-based perovskites CsSrX3 (XÂ=ÂCl, Br) under pressure for improved optoelectronic applications. Materials Today Communications, 2023, 34, 105188.	1.9	10
89	Theoretical prediction of thermal properties of \$\$hbox {YP}_{1-x}hbox {Sb}_{x}\$ alloys. Indian Journal of Physics, 0, , .	1.8	0
90	First-principles calculations to investigate the thermal response of the ZrC _(1â^'<i>x</i>) N _{<i>x</i>} ceramics at extreme conditions. High Temperature	1.4	0

#	Article	IF	CITATIONS
91	First principles calculations to investigate structural, electronic, mechanical, thermoelectric and optical properties of Bi- and Se-doped SnTe. Journal of Physics and Chemistry of Solids, 2023, 176, 111232.	4.0	3
92	First-principles calculations to investigate structural, electronic and optical properties of Cmc21-Ge2As2X (X = S, Se, Te and Po) under pressure effect. Journal of Physics and Chemistry of Solids, 2023, 176, 111231.	4.0	1
93	First-principles calculations to investigate probing the influence of Mn and Mg doping concentration on electronic structures and transport properties of SnTe alloys. Results in Physics, 2023, 48, 106443.	4.1	1
94	First-principles calculations to investigate electronic band structure, optical and mechanical properties of new CaFCl monolayer. Results in Physics, 2023, 45, 106251.	4.1	4
95	First-principles calculations to investigate structural, electronic, elastic and optical properties of radium based cubic fluoro-perovskite materials. Heliyon, 2023, 9, e13687.	3.2	2
96	First-principles calculations to investigate optical and electrical properties of the half-Heusler materials TiXSn (X = Ni, Pt). Molecular Simulation, 2023, 49, 778-791.	2.0	3
97	First-principles calculations to investigate structural, elastic and thermodynamic properties of new M2ScSnC2 (M=V or Nb) quaternary compounds for 312 MAX phases. Journal of Materials Research and Technology, 2023, 24, 3211-3221.	5.8	5
98	First-principles calculations to investigate optical properties of topological semimetal MX compounds (M = Ti, Zr, Hf and X = S, Se, Te). Materials Today Communications, 2023, 35, 106001.	1.9	2
99	First-principles calculations to investigate structural, electronic, and optical properties of zinc-blende CdxMg(1-x)TeyS(1- y) matched to CdX (X= S, Te) for Predicting critical thickness and corrective Term's effect. Solid State Communications, 2023, 368, 115189.	1.9	0
100	Unveiling the mechanical and dynamical stability to the contribution of transport properties of FeNbSb: A first principle approach. Computational Condensed Matter, 2023, 36, e00821.	2.1	2
101	First-principles calculations to investigate structural, elastic, electronic, and optical properties of XSrCl3 (X = Li, Na). Optik, 2023, 287, 171088.	2.9	4
102	First-Principles Calculations to Investigate Coupling Fe Doping with Oxygen Vacancies in Stannic Oxide and Their Physical Properties. Journal of Physical Chemistry C, 0, , .	3.1	2
103	First-principles calculations to investigate structural, electronic, magnetic, mechanical and thermodynamic properties of Half-Heusler alloy CoMnTe: Using GGA and GGA+U methods. Materials Chemistry and Physics, 2023, 307, 128115.	4.0	6
104	First-principles calculations to investigate structural, optical and electronic properties of ZrO ₂ , Zr _{0.93} Si _{0.07} O ₂ and Zr _{0.86} Si _{0.14} O ₂ for dye-sensitised solar cells applications. For the sensitised solar cells applications of Model and Mod	2.0	0
105	ZnFe <mml:math <br="" altimg="si5.svg" display="inline" xmlns:mml="http://www.w3.org/1998/Math/MathML">id="d1e1093"><mml:msub><mml:mrow /><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:mrow </mml:msub></mml:math> O <mml:math xmlns:mml="http://www.3.org/1998/Math/MathML" altimg="si6.svg" display="inline"</mml:math 	1.9	1
106	la= arterror > <mm:msub> <mm:mrow Investigation of structural /electronic; mechanical; & optisal characteristics of Ra based-cubic hydrides RbRaX3 (X= F and cl) perovskite materials for solar cell applications: First principle study. Heliyon, 2023, 9, e18407.</mm:mrow </mm:msub>	3.2	3
107	The stability, electronic, thermal, and optical properties of silver halide (AgX: X = F, Cl, Br, and I) semiconductors: Ab-initio study. Computational Condensed Matter, 2023, 37, e00837.	2.1	0
108	First-Principles Calculations to Investigate the Structural, Electronic, Optical, and Elastic Constants; Thermal Conductivity; Raman Scattering; Mulliken Population; and XPS Loss Features of Boron Nitride Polytypes. Journal of Physical Chemistry C, 2023, 127, 17213-17230.	3.1	2

#	Article	IF	CITATIONS
109	Static isotropic pressure induced semiconductor–metal transition and its impact on structural, electronic, elastic, mechanical and optical properties of SrCeO3. European Physical Journal Plus, 2023, 138, .	2.6	0
110	The new solid solution of double transition metal MXenes: Atomistic modeling of two-dimensional YScX (X= C and N). Solid State Sciences, 2023, 144, 107306.	3.2	2
111	First-principles calculations to investigate elastic properties, chemical bonds, electronic properties, magnetic properties, and phonon spectrum of CuNFe3 and CuNCo3. Journal of Materials Research and Technology, 2023, 26, 1798-1807.	5.8	1
112	lsotropic pressure induced structural, electronic, photocatalytic, elastic and mechanical properties of RbPbF ₃ : GGA-PBE and HSE03 based computational estimation. Physica Scripta, 2023, 98, 115913.	2.5	0
113	First-principles calculations to investigate electrochemical performance of the LiYO3 cathode for Li-ion battery. Ionics, 0, , .	2.4	1
114	Enhanced adsorption and sensitivity for SF6 decomposition gas detection on penta PdSe2 monolayer: A Density Functional Theory investigation with van der Waals correction. Materials Today Communications, 2023, 37, 107019.	1.9	1
115	Exploring the effects of external stress on the crystal lattice of SrHfO3: Significance of variations in structural, electrical, optical, and mechanical properties. Results in Optics, 2023, 13, 100519.	2.0	0
116	First-principles calculations to investigate stability, mechanical and thermo-dynamic properties of AlxTMy intermetallics in aluminum alloys. Solid State Communications, 2023, , 115361.	1.9	0
117	First-principles calculations to investigate the effect of X (X=B, Al, Ga) atomic substitution concentration on the electronic structure and optical properties of arsenene. Modern Physics Letters B, 0, , .	1.9	0
119	A DFT study of structural, electronic, optical, thermal and mechanical properties of cubic perovskite KGeX ₃ (X = Cl, Br) compound for solar cell applications. Physica Scripta, 2024, 99, 035922.	2.5	0
120	A comprehensive first-principles insights into the physical properties of binary intermetallic Zr3Ir compound. Results in Materials, 2024, 21, 100518.	1.8	0
121	First-principles calculations to investigate thermoelectric efficiency of β-In2S3 under pressure for renewable energy sources. Materials Science and Engineering B: Solid-State Materials for Advanced Technology, 2024, 301, 117183.	3.5	0