

Xudong Zhang

List of Publications by Year in descending order

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Version: 2024-02-01

37
papers

877
citations

394421

19
h-index

477307

29
g-index

37
all docs

37
docs citations

37
times ranked

216
citing authors

#	ARTICLE	IF	CITATIONS
1	Effect of structural vacancies on lattice vibration, mechanical, electronic, and thermodynamic properties of Cr ₅ BSi ₃ . Chinese Physics B, 2022, 31, 026101.	1.4	31
2	First-principles prediction of structure, mechanical and thermodynamic properties of Bi _x GeyOz ternary bismuth crystals. Vacuum, 2022, 195, 110696.	3.5	41
3	Exploring the electronic, mechanical, anisotropic, and optical properties of ternary silicides $\langle \text{TM} \rangle_2 \text{Si}_2 \text{Ys}$ ($\langle \text{TM} \rangle = \text{Cu, Ir, Os, Pt, Pd, Rh, Ru}$) from a first principles investigations. International Journal of Quantum Chemistry, 2022, 122, .	2.0	4
4	Exploring of the structural stability, mechanical, electronic and optical properties of hydrogenated RE ₅ Si ₄ (RE=Sc and Y) from first-principles calculations. Vacuum, 2022, 203, 111280.	3.5	3
5	The elasticity, anisotropy and thermodynamic properties of binary and ternary $\text{B} \llcorner \text{Sc}$ compounds: First-principles calculations. Solid State Communications, 2022, 353, 114869.	1.9	5
6	The vacancy defects and oxygen atoms occupation effects on mechanical and electronic properties of Mo ₅ Si ₃ silicides. Communications in Theoretical Physics, 2021, 73, 045702.	2.5	51
7	Insight into the structural stability and overall performances of V ₂ REAl ₂₀ ternary phases. Vacuum, 2021, 188, 110202.	3.5	0
8	The effects of vacancies defects and oxygen atoms occupation on physical properties of chromium silicide from a first-principles calculations. Solid State Communications, 2021, 340, 114535.	1.9	3
9	First-principles study of the lattice vibration, elastic anisotropy and thermodynamical properties of Tantalum Silicide with the different crystal structures. Vacuum, 2021, 191, 110410.	3.5	19
10	Investigation of the structural stability, mechanical, and thermodynamic properties of Hf ₅ BSi ₃ silicide with vacancies defects. Vacuum, 2021, 191, 110349.	3.5	15
11	The elastic anisotropy, electronic and thermodynamic properties of TM ₅ Si ₄ (TM= Sc, Y, Ti, Zr and Hf) silicides from first-principles calculations. Vacuum, 2021, 194, 110586.	3.5	15
12	Insight into the vacancy effects on mechanical and electronic properties of Tantalum Silicide. Ceramics International, 2020, 46, 4595-4601.	4.8	38
13	A first principles investigation on the influence of transition-metal elements on the structural, mechanical, and anisotropic properties of CaM ₂ Al ₂₀ intermetallics. Journal of Molecular Graphics and Modelling, 2020, 96, 107509.	2.4	43
14	Elastic anisotropy and thermodynamics properties of BiCu ₂ PO ₆ , BiZn ₂ PO ₆ and BiPb ₂ PO ₆ ceramics materials from first-principles calculations. Ceramics International, 2020, 46, 8575-8581.	4.8	26
15	First-principles investigation on the vacancy dependence on the optical and electronic properties of Bi ₂ S ₃ semiconductor ceramics. Vacuum, 2020, 181, 109759.	3.5	14
16	Insight into the vacancy effects on mechanical and electronic properties of V ₅ Si ₃ silicides from first-principles calculations. Journal of Molecular Graphics and Modelling, 2020, 98, 107600.	2.4	36
17	Insight into the structure dependence on physical properties of the high temperature ceramics TaB ₂ boride. Vacuum, 2020, 177, 109427.	3.5	26
18	The influence of vacancy defects on elastic and electronic properties of TaSi (5/3) desilicides from a first-principles calculations. Ceramics International, 2020, 46, 10992-10999.	4.8	59

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19	The mechanism of elastic and electronic properties of Tungsten Silicide (5/3) with vacancy defect from the first-principles calculations. <i>Vacuum</i> , 2020, 174, 109192.	3.5	20
20	Insight into the elastic anisotropy and thermodynamics properties of Tantalum borides. <i>Vacuum</i> , 2019, 169, 108883.	3.5	19
21	Insight into the pressure effect on the structural stability and physical properties of cubic sesquioxides X_2O_3 (X= Sc, Y and In). <i>Vacuum</i> , 2019, 168, 108855.	3.5	15
22	Theoretical prediction of new structure, mechanical properties, anisotropy in elasticity and thermodynamic properties of Mo_3Ge material. <i>Vacuum</i> , 2019, 170, 108978.	3.5	21
23	Phase stability, elastic, anisotropic and thermodynamic properties of $HoT_{2/3}Al_{20}$ ($T \in \{Ti, V, Cr\}$) intermetallic cage compounds. <i>Molecular Simulation</i> , 2019, 45, 833-840.	2.0	10
24	Insight into the elastic, electronic properties, anisotropy in elasticity of Manganese Borides. <i>Vacuum</i> , 2019, 165, 118-126.	3.5	58
25	Insight into the elastic anisotropy of BiM_2VO_6 (M= Mg, Ca and Cu) ceramics the first-principles calculations. <i>Vacuum</i> , 2019, 166, 26-31.	3.5	19
26	Insight into the elastic and anisotropic properties of $BiMg_2MO_6$ (M= P, As and V) ceramics from the first-principles calculations. <i>Ceramics International</i> , 2019, 45, 11136-11140.	4.8	34
27	First-principles investigation of the mechanical, anisotropic and thermodynamic properties of RE_2Al_{20} (RE=La, Ce, Gd, T=Ti, V) intermetallics. <i>Physica B: Condensed Matter</i> , 2019, 554, 64-71.	2.7	22
28	Structural, elastic, anisotropic and thermodynamic properties of the caged intermetallics $RETi_2Al_{20}$ (RE= La, Ce, Gd and Ho): A first-principles study. <i>Solid State Sciences</i> , 2019, 89, 121-129.	3.2	25
29	Anisotropy of the elasticity, thermal conductivity and optical parameters of $Cmcm$ and $Pm\bar{c}n$ $BiMg_2VO_6$ ceramics. <i>Vacuum</i> , 2019, 159, 218-227.	3.5	13
30	Phase stability, elastic, anisotropic properties, lattice dynamical and thermodynamic properties of $B_{12}M$ (M=Th, U, Np, Pu) dodecaborides. <i>Ceramics International</i> , 2018, 44, 128-135.	4.8	33
31	Phase stability, elastic, anisotropic and thermodynamic properties of GdT_2Al_{20} ($T \in \{Ti, V, Cr\}$) compounds: A first-principles study. <i>Vacuum</i> , 2018, 157, 312-319.	3.5	38
32	First-principles prediction of the physical properties of ThM_2Al_{20} (M= Ti, V, Cr) intermetallics. <i>Solid State Communications</i> , 2018, 284-286, 75-83.	1.9	38
33	First-Principles Investigation of Structural Stability, Mechanical, Anisotropic, and Thermodynamic Properties of $CeT_{2/3}Al_{20}$ Intermetallics. <i>Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences</i> , 2018, 73, 1157-1167.	1.5	5
34	Site preference of transition-metal elements additions on mechanical and electronic properties of B_2 DyCu-based alloys. <i>Materials and Design</i> , 2017, 133, 476-486.	7.0	29
35	Elastic, lattice dynamical, thermal stabilities and thermodynamic properties of BiF_3 -type Mg_3RE compounds from first-principles calculations. <i>Journal of Alloys and Compounds</i> , 2016, 663, 565-573.	5.5	29
36	First-principles investigation on the mechanical, vibrational and thermodynamics properties of $AuCu_3$ -type X_3Sc (X=Al, Ga, In) intermetallic compounds. <i>Computational Materials Science</i> , 2015, 106, 38-44.	3.0	14

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37	First-principle study of the physics properties of DO3â€Mg3Nd compound under high pressure. Superlattices and Microstructures, 2014, 73, 359-369.	3.1	6