Yong-Liang Guo

List of Publications by Year
in descending order

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39 papers	582 citations	687363 13 h-index	677142 22 g-index
39 all docs	39 docs citations	39 times ranked	465 citing authors

#	Article	IF	Citations
1	First-principles study of pressure-induced phase transitions, mechanical and thermodynamic properties of ThBC. Journal of Physics Condensed Matter, 2022, 34, 044001.	1.8	2
2	A computational study of strained MoS2 as catalysts for the electrocatalytic nitrogen reduction reaction. Journal of Molecular Structure, 2022, 1259, 132746.	3.6	10
3	Density functional theory study of N2 adsorption and dissociation on 3d transition metal atoms doped Ir(1 0 0) surface. Applied Surface Science, 2022, 597, 153678.	6.1	7
4	Density functional theory study of a two-atom active site transition-metal/iridium electrocatalyst for ammonia synthesis. Journal of Materials Chemistry A, 2022, 10, 13946-13957.	10.3	16
5	Stability, electronic, and mechanical properties of Si/Ge substitutionally doped T2CO2 (TÂ=ÂZr and Hf). Solid State Communications, 2022, 353, 114856.	1.9	3
6	Ab initio study on crystal structure and phase stability of ZrC2 under high pressure. Chinese Physics B, 2021, 30, 016101.	1.4	3
7	Density functional theory study of transition metal single-atoms anchored on graphyne as efficient electrocatalysts for the nitrogen reduction reaction. Physical Chemistry Chemical Physics, 2021, 23, 10418-10428.	2.8	68
8	First-principles study on Fe2B2 as efficient catalyst for nitrogen reduction reaction. Chinese Chemical Letters, 2021, 32, 3137-3142.	9.0	38
9	Strain-tunable electronic and optical properties of h-BN/BC₃ heterostructure with enhanced electron mobility*. Chinese Physics B, 2021, 30, 076801.	1.4	2
10	Computational Screening of 3â€‰d Transition Metal Atoms Anchored on Defective Graphene for Efficient Electrocatalytic N₂ Fixation. ChemPhysChem, 2021, 22, 1712-1721.	2.1	22
11	Crystal stabilities and electronic properties of thorium silicide under ambient conditions and high pressures from a first-principles study. Computational Materials Science, 2021, 197, 110561.	3.0	2
12	Electronic, mechanical and thermodynamic properties of ZrC, HfC and their solid solutions studied by first-principles calculation. Solid State Communications, 2021, 338, 114481.	1.9	9
13	Firstâ€Principles Study of 3d Transition Metal Atoms Doped Ni₁₃ Cluster as Efficient Electrocatalyst for Nitrogen Reduction Reaction. Advanced Theory and Simulations, 2021, 4, 2100353.	2.8	7
14	Theoretical Study on V Atom Supported on N and P-Doped Defective Graphene for Electrocatalytic Nitrogen Reduction. Journal of the Electrochemical Society, 2021, 168, 116516.	2.9	5
15	Prediction of structural and phase transitions of Th2CN from ambient pressure to 100 GPa: A first-principles study. Computational Materials Science, 2021, , 110980.	3.0	0
16	The effect of S-functionalized and vacancies on V2C MXenes as anode materials for Na-ion and Li-ion batteries. Current Applied Physics, 2020, 20, 310-319.	2.4	56
17	Study on the rolling friction and wear properties of surface densified powder metallurgy Fe-2Cu-0.6C material. Surface Topography: Metrology and Properties, 2020, 8, 015009.	1.6	5
18	First-principles study on crystal structures and superconductivity of molybdenum hydrides under high pressure. Journal of Applied Physics, 2020, 128, .	2.5	8

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19	Ab initio investigation of pressure-induced structural transitions and electronic evolution of Th3N4. High Pressure Research, 2020, 40, 267-282.	1.2	3
20	Effect of sulfur dopant atoms on the electronic band gap and optical properties of tin iodide. Chemical Physics Letters, 2019, 730, 557-561.	2.6	8
21	Stabilities and electronic properties of vacancy-doped Ti2CO2. Computational Materials Science, 2019, 159, 127-135.	3.0	21
22	Structural phase transitions and superconductivity of YC2 from first-principles calculations. Computational Materials Science, 2019, 159, 120-126.	3.0	4
23	Probing C3N/Graphene heterostructures as anode materials for Li-ion batteries. Journal of Power Sources, 2019, 413, 117-124.	7.8	68
24	Theoretical investigations of TiNbC MXenes as anode materials for Li-ion batteries. Journal of Alloys and Compounds, 2019, 778, 53-60.	5.5	49
25	Reversible hydrogen storage behaviors of Ti2N MXenes predicted by first-principles calculations. Journal of Materials Science, 2019, 54, 493-505.	3.7	38
26	First-principles study of the vibrational characteristics of the heavy element substitution on Cu3SbSe3. Computational Materials Science, 2019, 156, 167-174.	3.0	4
27	First-principles study on the phase transitions, crystal stabilities and thermodynamic properties of TiN under high pressure. Physics Letters, Section A: General, Atomic and Solid State Physics, 2018, 382, 656-661.	2.1	7
28	A First-Principles Study on the Vibrational and Electronic Properties of Zr-C MXenes. Communications in Theoretical Physics, 2018, 69, 336.	2.5	15
29	Elastic, mechanical, electronic, and defective properties of Zrâ€“Alâ€“C nanolaminates from first principles. Journal of the American Ceramic Society, 2018, 101, 756-772.	3.8	13
30	First-principles study on structural, mechanical and electronic properties of thorium dichalcogenides under high pressure. Journal of Nuclear Materials, 2018, 508, 147-153.	2.7	0
31	Theoretical study of mechanical, thermal and optical properties of (Ti1â^'xNb x)3AlC2 solid solutions. European Physical Journal B, 2018, 91, 1.	1.5	2
32	Structural Phase Transition of ThC Under High Pressure. Scientific Reports, 2017, 7, 96.	3.3	18
33	First-principles study of noble gas stability in ThO 2. Journal of Nuclear Materials, 2017, 490, 181-187.	2.7	13
34	First-principles study of fission product stability and clustering in ThO2. Computational Materials Science, 2017, 137, 186-194.	3.0	3
35	First-principles study of helium clustering at initial stage in ThO 2. Chinese Physics B, 2017, 26, 097101.	1.4	5
36	Pressure-induced structural transformations and polymerization in ThC2. Scientific Reports, 2017, 7, 45872.	3.3	13

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37	Structural and electronic phase transitions of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>ThS</mml:mi><mml:mn>2</mml:mn></mml:msub></m first-principles calculations. Physical Review B, 2016, 94, .	3.2	15
38	A new phase of ThC at high pressure predicted from a first-principles study. Physics Letters, Section A: General, Atomic and Solid State Physics, 2015, 379, 1607-1611.	2.1	17
39	First-principles study of the electronic structure and optical properties of defect chalcopyrite CdGa ₂ Te ₄. Chinese Physics B, 2012, 21, 123101.	1.4	7