Yong-Liang Guo

List of Publications by Year
in descending order

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Version: 2024-02-01

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	Probing C3N/Graphene heterostructures as anode materials for Li-ion batteries. Journal of Power Sources, 2019, 413, 117-124.	7.8	68
2	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
3	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
4	Theoretical investigations of TiNbC MXenes as anode materials for Li-ion batteries. Journal of Alloys and Compounds, 2019, 778, 53-60.	5.5	49
5	Reversible hydrogen storage behaviors of Ti2N MXenes predicted by first-principles calculations. Journal of Materials Science, 2019, 54, 493-505.	3.7	38
6	First-principles study on Fe2B2 as efficient catalyst for nitrogen reduction reaction. Chinese Chemical Letters, 2021, 32, 3137-3142.	9.0	38
7	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
8	Stabilities and electronic properties of vacancy-doped Ti2CO2. Computational Materials Science, 2019, 159, 127-135.	3.0	21
9	Structural Phase Transition of ThC Under High Pressure. Scientific Reports, 2017, 7, 96.	3.3	18
10	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
11	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
12	A First-Principles Study on the Vibrational and Electronic Properties of Zr-C MXenes. Communications in Theoretical Physics, 2018, 69, 336.	2.5	15
13	First-principles study of noble gas stability in ThO 2. Journal of Nuclear Materials, 2017, 490, 181-187.	2.7	13
14	Pressure-induced structural transformations and polymerization in ThC2. Scientific Reports, 2017, 7, 45872.	3.3	13
15	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
16	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></mm first-principles calculations. Physical Review B, 2016, 94, .	3.2	11
17	A computational study of strained MoS2 as catalysts for the electrocatalytic nitrogen reduction reaction. Journal of Molecular Structure, 2022, 1259, 132746.	3.6	10
18	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

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19	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
20	First-principles study on crystal structures and superconductivity of molybdenum hydrides under high pressure. Journal of Applied Physics, 2020, 128, .	2.5	8
21	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
22	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
23	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
24	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
25	First-principles study of helium clustering at initial stage in ThO 2. Chinese Physics B, 2017, 26, 097101.	1.4	5
26	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
27	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
28	Structural phase transitions and superconductivity of YC2 from first-principles calculations. Computational Materials Science, 2019, 159, 120-126.	3.0	4
29	First-principles study of the vibrational characteristics of the heavy element substitution on Cu3SbSe3. Computational Materials Science, 2019, 156, 167-174.	3.0	4
30	First-principles study of fission product stability and clustering in ThO2. Computational Materials Science, 2017, 137, 186-194.	3.0	3
31	Ab initio investigation of pressure-induced structural transitions and electronic evolution of Th3N4. High Pressure Research, 2020, 40, 267-282.	1.2	3
32	Ab initio study on crystal structure and phase stability of ZrC2 under high pressure. Chinese Physics B, 2021, 30, 016101.	1.4	3
33	Stability, electronic, and mechanical properties of Si/Ge substitutionally doped T2CO2 (TÂ=ÂZr and Hf). Solid State Communications, 2022, 353, 114856.	1.9	3
34	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
35	Strain-tunable electronic and optical properties of h-BN/BC₃ heterostructure with enhanced electron mobility*. Chinese Physics B, 2021, 30, 076801.	1.4	2
36	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

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37	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
38	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
39	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