

Yong-Liang Guo

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

36
papers

272
citations

10
h-index

15
g-index

39
ext. papers

424
ext. citations

3.4
avg, IF

4.07
L-index

#	Paper	IF	Citations
36	A computational study of strained MoS ₂ as catalysts for the electrocatalytic nitrogen reduction reaction. <i>Journal of Molecular Structure</i> , 2022 , 1259, 132746	3.4	0
35	Density functional theory study of N ₂ adsorption and dissociation on 3d transition metal atoms doped Ir(1 0 0) surface. <i>Applied Surface Science</i> , 2022 , 597, 153678	6.7	1
34	Theoretical Study on V Atom Supported on N and P-Doped Defective Graphene for Electrocatalytic Nitrogen Reduction. <i>Journal of the Electrochemical Society</i> , 2021 , 168, 116516	3.9	1
33	Prediction of structural and phase transitions of Th ₂ CN from ambient pressure to 100 GPa: A first-principles study. <i>Computational Materials Science</i> , 2021 , 110980	3.2	
32	Strain-tunable electronic and optical properties of h-BN/BC ₃ heterostructure with enhanced electron mobility*. <i>Chinese Physics B</i> , 2021 , 30, 076801	1.2	
31	Ab initio study on crystal structure and phase stability of ZrC ₂ under high pressure. <i>Chinese Physics B</i> , 2021 , 30, 016101	1.2	2
30	Density functional theory study of transition metal single-atoms anchored on graphyne as efficient electrocatalysts for the nitrogen reduction reaction. <i>Physical Chemistry Chemical Physics</i> , 2021 , 23, 10418-10428 ^{3,6}	10.428 ²⁰	
29	First-principles study on Fe ₂ B ₂ as efficient catalyst for nitrogen reduction reaction. <i>Chinese Chemical Letters</i> , 2021 , 32, 3137-3137	8.1	15
28	Computational Screening of 3 d Transition Metal Atoms Anchored on Defective Graphene for Efficient Electrocatalytic N Fixation. <i>ChemPhysChem</i> , 2021 , 22, 1712-1721	3.2	5
27	Crystal stabilities and electronic properties of thorium silicide under ambient conditions and high pressures from a first-principles study. <i>Computational Materials Science</i> , 2021 , 197, 110561	3.2	0
26	Electronic, mechanical and thermodynamic properties of ZrC, HfC and their solid solutions studied by first-principles calculation. <i>Solid State Communications</i> , 2021 , 338, 114481	1.6	1
25	First-principles study on crystal structures and superconductivity of molybdenum hydrides under high pressure. <i>Journal of Applied Physics</i> , 2020 , 128, 105901	2.5	5
24	Ab initio investigation of pressure-induced structural transitions and electronic evolution of Th ₃ N ₄ . <i>High Pressure Research</i> , 2020 , 40, 267-282	1.6	1
23	The effect of S-functionalized and vacancies on V ₂ C MXenes as anode materials for Na-ion and Li-ion batteries. <i>Current Applied Physics</i> , 2020 , 20, 310-319	2.6	29
22	Study on the rolling friction and wear properties of surface densified powder metallurgy Fe-2Cu-0.6C material. <i>Surface Topography: Metrology and Properties</i> , 2020 , 8, 015009	1.5	4
21	Effect of sulfur dopant atoms on the electronic band gap and optical properties of tin iodide. <i>Chemical Physics Letters</i> , 2019 , 730, 557-561	2.5	5
20	Stabilities and electronic properties of vacancy-doped Ti ₂ CO ₂ . <i>Computational Materials Science</i> , 2019 , 159, 127-135	3.2	10

19	Structural phase transitions and superconductivity of YC ₂ from first-principles calculations. <i>Computational Materials Science</i> , 2019 , 159, 120-126	3.2	3
18	Probing C ₃ N/Graphene heterostructures as anode materials for Li-ion batteries. <i>Journal of Power Sources</i> , 2019 , 413, 117-124	8.9	46
17	Theoretical investigations of TiNbC MXenes as anode materials for Li-ion batteries. <i>Journal of Alloys and Compounds</i> , 2019 , 778, 53-60	5.7	27
16	Reversible hydrogen storage behaviors of Ti ₂ N MXenes predicted by first-principles calculations. <i>Journal of Materials Science</i> , 2019 , 54, 493-505	4.3	15
15	First-principles study of the vibrational characteristics of the heavy element substitution on Cu ₃ SbSe ₃ . <i>Computational Materials Science</i> , 2019 , 156, 167-174	3.2	1
14	First-principles study on the phase transitions, crystal stabilities and thermodynamic properties of TiN under high pressure. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2018 , 382, 656-661	2.3	6
13	A First-Principles Study on the Vibrational and Electronic Properties of Zr-C MXenes. <i>Communications in Theoretical Physics</i> , 2018 , 69, 336	2.4	6
12	Elastic, mechanical, electronic, and defective properties of ZrAl ₂ C nanolaminates from first principles. <i>Journal of the American Ceramic Society</i> , 2018 , 101, 756-772	3.8	7
11	First-principles study on structural, mechanical and electronic properties of thorium dichalcogenides under high pressure. <i>Journal of Nuclear Materials</i> , 2018 , 508, 147-153	3.3	
10	Theoretical study of mechanical, thermal and optical properties of (Ti _{1-x} Nb _x) ₃ AlC ₂ solid solutions. <i>European Physical Journal B</i> , 2018 , 91, 1	1.2	2
9	Structural Phase Transition of ThC Under High Pressure. <i>Scientific Reports</i> , 2017 , 7, 96	4.9	12
8	First-principles study of noble gas stability in ThO ₂ . <i>Journal of Nuclear Materials</i> , 2017 , 490, 181-187	3.3	8
7	First-principles study of fission product stability and clustering in ThO ₂ . <i>Computational Materials Science</i> , 2017 , 137, 186-194	3.2	2
6	First-principles study of helium clustering at initial stage in ThO ₂ . <i>Chinese Physics B</i> , 2017 , 26, 097101	1.2	3
5	Pressure-induced structural transformations and polymerization in ThC. <i>Scientific Reports</i> , 2017 , 7, 45872	4.9	10
4	Structural and electronic phase transitions of ThS ₂ from first-principles calculations. <i>Physical Review B</i> , 2016 , 94,	3.3	7
3	A new phase of ThC at high pressure predicted from a first-principles study. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2015 , 379, 1607-1611	2.3	13
2	First-principles study of the electronic structure and optical properties of defect chalcopyrite CdGa ₂ Te ₄ . <i>Chinese Physics B</i> , 2012 , 21, 123101	1.2	4

- 1 First-Principles Study of 3d Transition Metal Atoms Doped Ni₁₃ Cluster as Efficient Electrocatalyst for Nitrogen Reduction Reaction. *Advanced Theory and Simulations*,2100353 3.5 ○