Yong-Liang Guo

List of Publications by Citations

36	272	10	15
papers	citations	h-index	g-index
39	424	3.4	4.07
ext. papers	ext. citations	avg, IF	L-index

#	Paper	IF	Citations
36	Probing C3N/Graphene heterostructures as anode materials for Li-ion batteries. *Journal of Power Sources*, **2019**, 413, 117-124	8.9	46
35	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	2.6	29
34	Theoretical investigations of TiNbC MXenes as anode materials for Li-ion batteries. *Journal of Alloys and Compounds*, **2019**, 778, 53-60	5.7	27
33	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	3.6	20
32	Reversible hydrogen storage behaviors of Ti2N MXenes predicted by first-principles calculations. *Journal of Materials Science*, **2019**, 54, 493-505	4.3	15
31	First-principles study on Fe2B2 as efficient catalyst for nitrogen reduction reaction. *Chinese Chemical Letters*, **2021**, 32, 3137-3137	8.1	15
30	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	2.3	13
29	Structural Phase Transition of ThC Under High Pressure. *Scientific Reports*, **2017**, 7, 96	4.9	12
28	Pressure-induced structural transformations and polymerization in ThC. *Scientific Reports*, **2017**, 7, 45872	4.9	10
27	Stabilities and electronic properties of vacancy-doped Ti2CO2. *Computational Materials Science*, **2019**, 159, 127-135	3.2	10
26	First-principles study of noble gas stability in ThO 2. *Journal of Nuclear Materials*, **2017**, 490, 181-187	3.3	8
25	Elastic, mechanical, electronic, and defective properties of Zr$_4$AlC$_3$ nanolaminates from first principles. *Journal of the American Ceramic Society*, **2018**, 101, 756-772	3.8	7
24	Structural and electronic phase transitions of ThS2 from first-principles calculations. *Physical Review B*, **2016**, 94,	3.3	7
23	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	2.3	6
22	A First-Principles Study on the Vibrational and Electronic Properties of Zr-C MXenes. *Communications in Theoretical Physics*, **2018**, 69, 336	2.4	6
21	Effect of sulfur dopant atoms on the electronic band gap and optical properties of tin iodide. *Chemical Physics Letters*, **2019**, 730, 557-561	2.5	5
20	First-principles study on crystal structures and superconductivity of molybdenum hydrides under high pressure. *Journal of Applied Physics*, **2020**, 128, 105901	2.5	5

19	Computational Screening of 3 d Transition Metal Atoms Anchored on Defective Graphene for Efficient Electrocatalytic N Fixation. *ChemPhysChem*, **2021**, 22, 1712-1721	3.2	5
18	First-principles study of the electronic structure and optical properties of defect chalcopyrite CdGa 2 Te 4. *Chinese Physics B*, **2012**, 21, 123101	1.2	4
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	1.5	4
16	First-principles study of helium clustering at initial stage in ThO 2. *Chinese Physics B*, **2017**, 26, 097101	1.2	3
15	Structural phase transitions and superconductivity of YC2 from first-principles calculations. *Computational Materials Science*, **2019**, 159, 120-126	3.2	3
14	First-principles study of fission product stability and clustering in ThO2. *Computational Materials Science*, **2017**, 137, 186-194	3.2	2
13	Ab initio study on crystal structure and phase stability of ZrC2 under high pressure. *Chinese Physics B*, **2021**, 30, 016101	1.2	2
12	Theoretical study of mechanical, thermal and optical properties of (Ti1⊠Nb x)3AlC2 solid solutions. *European Physical Journal B*, **2018**, 91, 1	1.2	2
11	Ab initio investigation of pressure-induced structural transitions and electronic evolution of Th3N4. *High Pressure Research*, **2020**, 40, 267-282	1.6	1
10	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	3.9	1
9	First-principles study of the vibrational characteristics of the heavy element substitution on Cu3SbSe3. *Computational Materials Science*, **2019**, 156, 167-174	3.2	1
8	Electronic, mechanical and thermodynamic properties of ZrC, HfC and their solid solutions studied by first-principles calculation. *Solid State Communications*, **2021**, 338, 114481	1.6	1
7	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	6.7	1
6	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	0
5	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	3.2	0
4	A computational study of strained MoS2 as catalysts for the electrocatalytic nitrogen reduction reaction. *Journal of Molecular Structure*, **2022**, 1259, 132746	3.4	0
3	Prediction of structural and phase transitions of Th2CN from ambient pressure to 100 GPa: A first-principles study. *Computational Materials Science*, **2021**, 110980	3.2	
2	Strain-tunable electronic and optical properties of h-BN/BC3 heterostructure with enhanced electron mobility*. *Chinese Physics B*, **2021**, 30, 076801	1.2	

1 First-principles study on structural, mechanical and electronic properties of thorium dichalcogenides under high pressure. *Journal of Nuclear Materials*, **2018**, 508, 147-153 3.3