Guo-Xu Zhang

List of Publications by Year
in descending order

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18 papers	1,852 citations	759233 12 h-index	888059 17 g-index
18 all docs	18 docs citations	18 times ranked	3577 citing authors

#	Article	IF	Citations
1	Structural phase transition of monochalcogenides investigated with machine learning. Physical Review B, 2022, 105, .	3.2	7
2	Magnetic phase transition of monolayer chromium trihalides investigated with machine learning: toward a universal magnetic Hamiltonian. Journal of Physics Condensed Matter, 2022, 34, 395901.	1.8	1
3	Surface Strain-Induced Collective Switching of Ensembles of Molecules on Metal Surfaces. Journal of Physical Chemistry Letters, 2020, 11, 2277-2283.	4.6	4
4	Graphite Nâ€“Câ€“P dominated three-dimensional nitrogen and phosphorus co-doped holey graphene foams as high-efficiency electrocatalysts for Znâ€“air batteries. Nanoscale, 2019, 11, 17010-17017.	5.6	48
5	Surface modification of Li1.2Mn0.54Ni0.13Co0.13O2 via an ionic conductive LiV3O8 as a cathode material for Li-ion batteries. Ionics, 2019, 25, 4567-4576.	2.4	11
6	Single metal atoms regulated flexibly by a 2D InSe substrate for CO₂ reduction electrocatalysts. Journal of Materials Chemistry A, 2019, 7, 8210-8217.	10.3	26
7	Electroreduction of CO₂ on Cu Clusters: The Effects of Size, Symmetry, and Temperature. ChemElectroChem, 2019, 6, 1831-1837.	3.4	36
8	Performance of various density-functional approximations for cohesive properties of 64 bulk solids. New Journal of Physics, 2018, 20, 063020.	2.9	185
9	Reproducibility in density functional theory calculations of solids. Science, 2016, 351, aad3000.	12.6	1,113
10	First-principles study on the electronic and bonding properties of PbTiO3 (110) polar terminations. Chemical Research in Chinese Universities, 2015, 31, 825-829.	2.6	1
11	A first-principles investigation of the stabilities and electronic properties of SrZrO₃(1â€‰1â€‰0)(1â€‰Ã—â€‰1) polar terminations. Journal of Physics Condensed Matter, 2014, 26, 395002.	1.8	13
12	Electrodynamic response and stability of molecular crystals. Physical Review B, 2013, 87, .	3.2	40
13	Structure and energetics of benzene adsorbed on transition-metal surfaces: density-functional theory with van der Waals interactions including collective substrate response. New Journal of Physics, 2013, 15, 053046.	2.9	143
14	van der Waals Interactions in Ionic and Semiconductor Solids. Physical Review Letters, 2011, 107, 245501.	7.8	143
15	Firstâ€principles calculations of the stability and electronic properties of the PbTiO₃ (110) polar surface. Journal of Computational Chemistry, 2009, 30, 1785-1798.	3.3	18
16	Lattice dynamics investigation of different transition behaviors of cubic BaTiO₃and SrTiO₃by first-principles calculations. Journal of Physics Condensed Matter, 2008, 20, 215215.	1.8	25
17	A first-principles investigation into the ferroelectric and antiferrodistortive instabilities of cubic SrTiO₃. Journal of Physics Condensed Matter, 2007, 19, 506213.	1.8	6
18	First-Principles Investigation of Stability and Structural Properties of the BaTiO3(110) Polar Surface. Journal of Physical Chemistry C, 2007, 111, 6343-6349.	3.1	32