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	Reproducibility in density functional theory calculations of solids. Science, 2016, 351, aad3000.	12.6	1,113
2	Performance of various density-functional approximations for cohesive properties of 64 bulk solids. New Journal of Physics, 2018, 20, 063020.	2.9	185
3	van der Waals Interactions in Ionic and Semiconductor Solids. Physical Review Letters, 2011, 107, 245501.	7.8	143
4	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
5	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
6	Electrodynamic response and stability of molecular crystals. Physical Review B, 2013, 87, .	3.2	40
7	Electroreduction of CO₂ on Cu Clusters: The Effects of Size, Symmetry, and Temperature. ChemElectroChem, 2019, 6, 1831-1837.	3.4	36
8	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
9	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
10	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
11	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
12	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
13	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
14	Structural phase transition of monochalcogenides investigated with machine learning. Physical Review B, 2022, 105, .	3.2	7
15	A first-principles investigation into the ferroelectric and antiferrodistortive instabilities of cubic SrTiO₃. Journal of Physics Condensed Matter, 2007, 19, 506213.	1.8	6
16	Surface Strain-Induced Collective Switching of Ensembles of Molecules on Metal Surfaces. Journal of Physical Chemistry Letters, 2020, 11, 2277-2283.	4.6	4
17	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
18	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