Yubo Zhang

List of Publications by Year in descending order

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41 papers	3,674 citations	304368 22 h-index	315357 38 g-index
43 all docs	43 docs citations	43 times ranked	6259 citing authors

#	Article	IF	Citations
1	Accurate first-principles structures and energies of diversely bonded systems from an efficient density functional. Nature Chemistry, 2016, 8, 831-836.	6.6	698
2	Enhanced performance of light-controlled conductive switching in hybrid cuprous oxide/reduced graphene oxide (Cu_2O/rGO) nanocomposites. Optics Letters, 2017, 42, 911.	1.7	551
3	Enhanced photoresponse of self-powered perovskite photodetector based on ZnO nanoparticles decorated CsPbBr3 films. Solar Energy Materials and Solar Cells, 2017, 172, 341-346.	3.0	408
4	Highâ€Performance Pseudocubic Thermoelectric Materials from Nonâ€cubic Chalcopyrite Compounds. Advanced Materials, 2014, 26, 3848-3853.	11.1	269
5	Theoretical and experimental investigation of highly photocatalytic performance of CuInZnS nanoporous structure for removing the NO gas. Journal of Catalysis, 2018, 357, 100-107.	3.1	214
6	High intrinsic carrier mobility and photon absorption in the perovskite CH₃NH₃PbI₃. Physical Chemistry Chemical Physics, 2015, 17, 11516-11520.	1.3	182
7	Efficient first-principles prediction of solid stability: Towards chemical accuracy. Npj Computational Materials, 2018, 4, .	3.5	157
8	Comparative first-principles studies of prototypical ferroelectric materials by LDA, GGA, and SCAN meta-GGA. Physical Review B, 2017, 96, .	1.1	156
9	Comparative study of structural and electronic properties of Cu-based multinary semiconductors. Physical Review B, 2011, 84, .	1.1	95
10	An accurate first-principles treatment of doping-dependent electronic structure of high-temperature cuprate superconductors. Communications Physics, 2018, 1, .	2.0	94
11	Antiferromagnetic ground state of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>La</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math>CuO₄: A parameter-free ab initio description. Physical Review B, 2018, 98, .	1.1	80
12	Structural properties and quasiparticle band structures of Cu-based quaternary semiconductors for photovoltaic applications. Journal of Applied Physics, 2012, 111, .	1.1	67
13	Screened Coulomb interaction of localized electrons in solids from first principles. Physical Review B, 2012, 85, .	1.1	62
14	Competing stripe and magnetic phases in the cuprates from first principles. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 68-72.	3.3	61
15	Regulating Excitonâ€“Phonon Coupling to Achieve a Nearâ€Unity Photoluminescence Quantum Yield in Oneâ€Dimensional Hybrid Metal Halides. Advanced Science, 2021, 8, e2100786.	5.6	61
16	Electronic structure of antifluorite Cu2X (X = S, Se, Te) within the modified Becke-Johnson potential plus an on-site Coulomb U. Journal of Chemical Physics, 2014, 140, 074702.	1.2	58
17	VO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>: Orbital competition, magnetism, and phase stability. Physical Review B, 2012, 86, .	1.1	53
18	Electronic properties of energy harvesting Cu-chalcogenides: pâ€“d hybridization and d-electron localization. Computational Materials Science, 2015, 108, 239-249.	1.4	49

#	Article	IF	Citations
19	Symmetry-breaking polymorphous descriptions for correlated materials without interelectronic U. Physical Review B, 2020, 102, .	1.1	48
20	Near-edge band structures and band gaps of Cu-based semiconductors predicted by the modified Becke-Johnson potential plus an on-site Coulomb U. Journal of Chemical Physics, 2013, 139, 184706.	1.2	43
21	High photodegradation efficiency of Rhodamine B catalyzed by bismuth silicate nanoparticles. Catalysis Communications, 2013, 39, 65-69.	1.6	33
22	Subtlety of TiO2 phase stability: Reliability of the density functional theory predictions and persistence of the self-interaction error. Journal of Chemical Physics, 2019, 150, 014105.	1.2	32
23	Exceptionally large anomalous Hall effect due to anticrossing of spin-split bands in the antiferromagnetic half-Heusler compound TbPtBi. Physical Review B, 2020, 101, .	1.1	24
24	First-principles calculation of spin and orbital contributions to magnetically ordered moments in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Sr</mml:mi><mml:mn>2</mml:mn></mml:r Physical Review B, 2020, 101, .	1.1	23
25	Half-Heusler-like compounds with wide continuous compositions and tunable p- to n-type semiconducting thermoelectrics. Nature Communications, 2022, 13, 35.	5.8	20
26	Pinning down high-performance Cu-chalcogenides as thin-film solar cell absorbers: A successive screening approach. Journal of Chemical Physics, 2016, 144, 194706.	1.2	18
27	Thermodynamic Ground States of Multifunctional Metal Dodecaborides. Chemistry of Materials, 2019, 31, 1075-1083.	3.2	15
28	Effects of biaxial strain on the improper multiferroicity inhâ"LuFeO3films studied using the restrained thermal expansion method. Physical Review B, 2017, 95, .	1.1	14
29	Spinon excitations in the quasi-one-dimensional <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>S</mml:mi><mml:mo>=</mml:mo><mml:mfrac><mml chain compound <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi mathvariant="normal">C</mml:mi><mml:msub><mml:mi mathvariant="normal">s</mml:mi><mml:mn>4</mml:mn></mml:msub><mml:mi>CuS</mml:mi><mml:msub><mml:mi mathvariant="normal">b</mml:mi><mml:mn>. Physical Review B, 2020, 101, .	1.1	14
30	Tunable catalytic activity of cobalt-intercalated layered MnO2 for water oxidation through confinement and local ordering. Journal of Catalysis, 2019, 374, 143-149.	3.1	13
31	First-principles study of the halide-passivation effects on the electronic structures of CdSe quantum dots. RSC Advances, 2014, 4, 19302-19309.	1.7	12
32	Sensitivity of the electronic and magnetic structures of cuprate superconductors to density functional approximations. Npj Computational Materials, 2022, 8, .	3.5	12
33	Remarkable Band-Gap Renormalization via Dimensionality of the Layered Material <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" overflow="scroll"><mml:msub><mml:mrow><mml:mrow><mml:mi mathvariant="normal">C</mml:mi></mml:mrow></mml:mrow><mml:mn>3</mml:mn></mml:msub><mml:mrow><mml:mrow><mml:mi mathvariant="normal">B</mml:mi></mml:mrow></mml:mrow></mml:math>. Physical Review Applied, 2020, 14.	1.5	9
34	Localization in the SCAN meta-generalized gradient approximation functional leading to broken symmetry ground states for graphene and benzene. Physical Chemistry Chemical Physics, 2020, 22, 19585-19591.	1.3	8
35	Density functional theory. , 2019, , 119-159.		7
36	Critical role of magnetic moments in heavy-fermion materials: Revisiting <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow><mml:mi>SmB</mml:mi></mml:mrow><mml:mn>6</mml:mn></mml:r Physical Review B, 2022, 105, .	1.1	6

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37	Quasiparticle band structures of IIâ€“VI semiconductors containing semicore states in the approach. Solid State Communications, 2012, 152, 588-592.	0.9	5
38	Magnetic oxygen in transition metal oxides: A case study of Ba2CoO4. Journal of Physics and Chemistry of Solids, 2021, 150, 109803.	1.9	2
39	Strong excitonic effect in organicâ€“inorganic hybrid crystals. Solid State Communications, 2012, 152, 1259-1262.	0.9	1
40	Geometry strategy for engineering the recombination possibility of excitons in nanowires. Nanoscale, 2016, 8, 7318-7325.	2.8	0
41	Identification of a monoclinic metallic state in VO2 from a modified first-principles approach. Modern Physics Letters B, 2019, 33, 1950148.	1.0	0