

Yubo Zhang

List of Publications by Year in descending order

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41
papers

3,674
citations

304368

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315357

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43
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43
docs citations

43
times ranked

6259
citing authors

#	ARTICLE	IF	CITATIONS
1	Half-Heusler-like compounds with wide continuous compositions and tunable p- to n-type semiconducting thermoelectrics. Nature Communications, 2022, 13, 35.	5.8	20
2	Sensitivity of the electronic and magnetic structures of cuprate superconductors to density functional approximations. Npj Computational Materials, 2022, 8, .	3.5	12
3	Critical role of magnetic moments in heavy-fermion materials: Revisiting SmB_6 . Physical Review B, 2022, 105, .		6
4	Magnetic oxygen in transition metal oxides: A case study of Ba_2CoO_4 . Journal of Physics and Chemistry of Solids, 2021, 150, 109803.	1.9	2
5	Regulating Exciton-Phonon Coupling to Achieve a Near-Unity Photoluminescence Quantum Yield in One-Dimensional Hybrid Metal Halides. Advanced Science, 2021, 8, e2100786.	5.6	61
6	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
7	Symmetry-breaking polymorphous descriptions for correlated materials without interelectronic $\langle i \rangle U \langle j \rangle$. Physical Review B, 2020, 102, .	1.1	48
8	Remarkable Band-Gap Renormalization via Dimensionality of the Layered Material C_3B_2 . Physical Review Applied, 2020, 14, .	1.5	9
9	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
10	Spinon excitations in the quasi-one-dimensional S_1C_3 chain compound C_3B_2 . Physical Review Applied, 2020, 14, .	1.1	14
11	First-principles calculation of spin and orbital contributions to magnetically ordered moments in Sr_2CuO_7 . Physical Review B, 2020, 101, .	1.1	23
12	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
13	Tunable catalytic activity of cobalt-intercalated layered MnO_2 for water oxidation through confinement and local ordering. Journal of Catalysis, 2019, 374, 143-149.	3.1	13
14	Identification of a monoclinic metallic state in VO_2 from a modified first-principles approach. Modern Physics Letters B, 2019, 33, 1950148.	1.0	0
15	Thermodynamic Ground States of Multifunctional Metal Dodecaborides. Chemistry of Materials, 2019, 31, 1075-1083.	3.2	15
16	Subtlety of TiO_2 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
17	Density functional theory. , 2019, , 119-159.		7
18	An accurate first-principles treatment of doping-dependent electronic structure of high-temperature cuprate superconductors. Communications Physics, 2018, 1, .	2.0	94

#	ARTICLE	IF	CITATIONS
19	Efficient first-principles prediction of solid stability: Towards chemical accuracy. Npj Computational Materials, 2018, 4, .	3.5	157
20	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
21	Antiferromagnetic ground state of La_2CuO_4 : A parameter-free <i>ab initio</i> description. Physical Review B, 2018, 98, .	2.1	80
22	Effects of biaxial strain on the improper multiferroicity in LuFeO_3 films studied using the restrained thermal expansion method. Physical Review B, 2017, 95, .	1.1	14
23	Enhanced photoresponse of self-powered perovskite photodetector based on ZnO nanoparticles decorated CsPbBr ₃ films. Solar Energy Materials and Solar Cells, 2017, 172, 341-346.	3.0	408
24	Comparative first-principles studies of prototypical ferroelectric materials by LDA, GGA, and SCAN meta-GGA. Physical Review B, 2017, 96, .	1.1	156
25	Enhanced performance of light-controlled conductive switching in hybrid cuprous oxide/reduced graphene oxide (Cu ₂ O/rGO) nanocomposites. Optics Letters, 2017, 42, 911.	1.7	551
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	Accurate first-principles structures and energies of diversely bonded systems from an efficient density functional. Nature Chemistry, 2016, 8, 831-836.	6.6	698
28	Geometry strategy for engineering the recombination possibility of excitons in nanowires. Nanoscale, 2016, 8, 7318-7325.	2.8	0
29	Electronic properties of energy harvesting Cu-chalcogenides: <i>d</i> hybridization and <i>d</i> -electron localization. Computational Materials Science, 2015, 108, 239-249.	1.4	49
30	High intrinsic carrier mobility and photon absorption in the perovskite $\text{CH}_3\text{NH}_3\text{PbI}_3$. Physical Chemistry Chemical Physics, 2015, 17, 11516-11520.	1.3	182
31	Electronic structure of antifluorite Cu_2X (X = S, Se, Te) within the modified Becke-Johnson potential plus an on-site Coulomb <i>U</i> . Journal of Chemical Physics, 2014, 140, 074702.	1.2	58
32	High-Performance Pseudocubic Thermoelectric Materials from Non-cubic Chalcopyrite Compounds. Advanced Materials, 2014, 26, 3848-3853.	11.1	269
33	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
34	Near-edge band structures and band gaps of Cu-based semiconductors predicted by the modified Becke-Johnson potential plus an on-site Coulomb <i>U</i> . Journal of Chemical Physics, 2013, 139, 184706.	1.2	43
35	High photodegradation efficiency of Rhodamine B catalyzed by bismuth silicate nanoparticles. Catalysis Communications, 2013, 39, 65-69.	1.6	33
36	Screened Coulomb interaction of localized electrons in solids from first principles. Physical Review B, 2012, 85, .	1.1	62

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37	VO $\langle \text{mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"} \langle \text{mml:msub} \langle \text{mml:mrow} / \rangle \langle \text{mml:mn} \rangle 2 \langle \text{mml:mn} \rangle \langle \text{mml:msub} \rangle \langle \text{mml:math} \rangle$: Orbital competition, magnetism, and phase stability. Physical Review B, 2012, 86, .	1.1	53
38	Structural properties and quasiparticle band structures of Cu-based quaternary semiconductors for photovoltaic applications. Journal of Applied Physics, 2012, 111, .	1.1	67
39	Quasiparticle band structures of II-VI semiconductors containing semicore states in the approach. Solid State Communications, 2012, 152, 588-592.	0.9	5
40	Strong excitonic effect in organic-inorganic hybrid crystals. Solid State Communications, 2012, 152, 1259-1262.	0.9	1
41	Comparative study of structural and electronic properties of Cu-based multinary semiconductors. Physical Review B, 2011, 84, .	1.1	95