Qiang Zhu

List of Publications by Year
in descending order

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60 papers	5,490 citations	147801 31 h-index	133252 59 g-index
61 all docs	61 docs citations	61 times ranked	5806 citing authors

#	Article	IF	Citations
1	Modeling surface spin polarization on ceria-supported Pt nanoparticles. Journal of Physics Condensed Matter, 2022, , .	1.8	0
2	PyXtal_FF: a python library for automated force field generation. Machine Learning: Science and Technology, 2021, 2, 027001.	5.0	18
3	Computation and data driven discovery of topological phononic materials. Nature Communications, 2021, 12, 1204.	12.8	98
4	Switchable two-dimensional electrides: A first-principles study. Physical Review B, 2021, 103, .	3.2	9
5	PyXtal: A Python library for crystal structure generation and symmetry analysis. Computer Physics Communications, 2021, 261, 107810.	7.5	40
6	Tunable Contacts in Graphene/InSe van der Waals Heterostructures. Journal of Physical Chemistry C, 2020, 124, 23699-23706.	3.1	25
7	Neural network potential from bispectrum components: A case study on crystalline silicon. Journal of Chemical Physics, 2020, 153, 054118.	3.0	12
8	Spectral neural network potentials for binary alloys. Journal of Applied Physics, 2020, 128, 045113.	2.5	4
9	High dielectric ternary oxides from crystal structure prediction and high-throughput screening. Scientific Data, 2020, 7, 81.	5.3	9
10	A Revisited Mechanism of the Graphite-to-Diamond Transition at High Temperature. Matter, 2020, 3, 864-878.	10.0	30
11	Computational Discovery of Inorganic Electrides from an Automated Screening. Matter, 2019, 1, 1293-1303.	10.0	42
12	Electrides with Dinitrogen Ligands. ACS Applied Materials & Interfaces, 2019, 11, 5256-5263.	8.0	15
13	Superconductivity in the van der Waals layered compound PS2. Physical Review B, 2019, 99, .	3.2	11
14	Magnetic borophenes from an evolutionary search. Physical Review B, 2019, 99, .	3.2	25
15	First-principles studies of a two-dimensional electron gas at the interface of polar/polar LaAlO₃/KNbO₃ superlattices. Physical Chemistry Chemical Physics, 2019, 21, 8046-8053.	2.8	9
16	Structure prediction drives materials discovery. Nature Reviews Materials, 2019, 4, 331-348.	48.7	402
17	Inverse Correlation between Lethality and Thermodynamic Stability of Contact Insecticide Polymorphs. Crystal Growth and Design, 2019, 19, 1839-1844.	3.0	18
18	Ternary inorganic electrides with mixed bonding. Physical Review B, 2019, 99, .	3.2	26

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19	Structure-Controlled Oxygen Concentration in Fe₂O₃ and FeO₂. Inorganic Chemistry, 2019, 58, 5476-5482.	4.0	10
20	Computational design of flexible electrides with nontrivial band topology. Physical Review Materials, 2019, 3, .	2.4	18
21	Grain boundary phases in bcc metals. Nanoscale, 2018, 10, 8253-8268.	5.6	55
22	Predicting phase behavior of grain boundaries with evolutionary search and machine learning. Nature Communications, 2018, 9, 467.	12.8	122
23	Predicting the ground-state structure of sodium boride. Physical Review B, 2018, 97, .	3.2	26
24	The stability and unexpected chemistry of oxide clusters. Physical Chemistry Chemical Physics, 2018, 20, 30437-30444.	2.8	11
25	Boron oxides under pressure: Prediction of the hardest oxides. Physical Review B, 2018, 98, .	3.2	18
26	First-principles investigation of Sc-III/IV under high pressure. Physical Review B, 2018, 98, .	3.2	12
27	Crystal structure evaluation: calculating relative stabilities and other criteria: general discussion. Faraday Discussions, 2018, 211, 325-381.	3.2	7
28	Applications of crystal structure prediction â€“ organic molecular structures: general discussion. Faraday Discussions, 2018, 211, 493-539.	3.2	8
29	Pressure-induced structural phase transition in Li4Ge. CrystEngComm, 2018, 20, 5949-5954.	2.6	2
30	Oligomer Hydrate Crystallization Improves Carbon Nanotube Memory. Chemistry of Materials, 2018, 30, 3813-3818.	6.7	6
31	ROY revisited, again: the eighth solved structure. Faraday Discussions, 2018, 211, 477-491.	3.2	55
32	Structures and transitions in bcc tungsten grain boundaries and their role in the absorption of point defects. Acta Materialia, 2018, 159, 123-134.	7.9	44
33	Pressure-induced structural and electronic transitions, metallization, and enhanced visible-light responsiveness in layered rhenium disulphide. Physical Review B, 2018, 97, .	3.2	35
34	The Structure of Glycine Dihydrate: Implications for the Crystallization of Glycine from Solution and Its Structure in Outer Space. Angewandte Chemie - International Edition, 2017, 56, 2030-2034.	13.8	35
35	A stable compound of helium and sodium at high pressure. Nature Chemistry, 2017, 9, 440-445.	13.6	276
36	The Structure of Glycine Dihydrate: Implications for the Crystallization of Glycine from Solution and Its Structure in Outer Space. Angewandte Chemie, 2017, 129, 2062-2066.	2.0	14

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37	Powder diffraction and crystal structure prediction identify four new coumarin polymorphs. Chemical Science, 2017, 8, 4926-4940.	7.4	97
38	The Third Ambient Aspirin Polymorph. Crystal Growth and Design, 2017, 17, 3562-3566.	3.0	73
39	DDT Polymorphism and the Lethality of Crystal Forms. Angewandte Chemie - International Edition, 2017, 56, 10165-10169.	13.8	46
40	DDT Polymorphism and the Lethality of Crystal Forms. Angewandte Chemie, 2017, 129, 10299-10303.	2.0	21
41	The unexpectedly rich reconstructions of rutile TiO2(011)-(2 Ã— 1) surface and the driving forces behind their formation: an ab initio evolutionary study. Physical Chemistry Chemical Physics, 2016, 18, 19549-19556.	2.8	18
42	Report on the sixth blind test of organic crystal structure prediction methods. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2016, 72, 439-459.	1.1	445
43	Resorcinol Crystallization from the Melt: A New Ambient Phase and New â€œRiddlesâ€• Journal of the American Chemical Society, 2016, 138, 4881-4889.	13.7	74
44	Stable magnesium peroxide at high pressure. Scientific Reports, 2015, 5, 13582.	3.3	30
45	Generalized evolutionary metadynamics for sampling the energy landscapes and its applications. Physical Review B, 2015, 92, .	3.2	33
46	New Reconstructions of the (110) Surface of Rutile<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>TiO</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn></m by an Evolutionary Method. Physical Review Letters, 2014, 113, 266101.	7.8	61
47	Semimetallic Two-Dimensional Boron Allotrope with Massless Dirac Fermions. Physical Review Letters, 2014, 112, .	7.8	497
48	Predicting polymeric crystal structures by evolutionary algorithms. Journal of Chemical Physics, 2014, 141, 154102.	3.0	41
49	Variable-composition structural optimization and experimental verification of MnB₃and MnB₄. Physical Chemistry Chemical Physics, 2014, 16, 15866-15873.	2.8	49
50	Rational design of all organic polymer dielectrics. Nature Communications, 2014, 5, 4845.	12.8	259
51	Unexpected Stable Stoichiometries of Sodium Chlorides. Science, 2013, 342, 1502-1505.	12.6	394
52	Stability of xenon oxides at high pressures. Nature Chemistry, 2013, 5, 61-65.	13.6	118
53	New developments in evolutionary structure prediction algorithm USPEX. Computer Physics Communications, 2013, 184, 1172-1182.	7.5	1,031
54	Novel stable compounds in the Mgâ€“O system under high pressure. Physical Chemistry Chemical Physics, 2013, 15, 7696.	2.8	102

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55	Evolutionary method for predicting surface reconstructions with variable stoichiometry. Physical Review B, 2013, 87, .	3.2	99
56	First-Principles Determination of the Structure of Magnesium Borohydride. Physical Review Letters, 2012, 109, 245503.	7.8	47
57	Systematic search for low-enthalpy<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>s</mml:mi><mml:msup><mml:mi>p</mml:mi><mml:mn>3</mml:mn></mml:msup></mml:mrow></mml:math> allotropes using evolutionary metadynamics. Physical Review B, 2012, 85, .	3.2	82
58	Evolutionary metadynamics: a novel method to predict crystal structures. CrystEngComm, 2012, 14, 3596.	2.6	62
59	Constrained evolutionary algorithm for structure prediction of molecular crystals: methodology and applications. Acta Crystallographica Section B: Structural Science, 2012, 68, 215-226.	1.8	146
60	Denser than diamond:Ab initiosearch for superdense carbon allotropes. Physical Review B, 2011, 83, .	3.2	118