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	New developments in evolutionary structure prediction algorithm USPEX. Computer Physics Communications, 2013, 184, 1172-1182.	7.5	1,031
2	Semimetallic Two-Dimensional Boron Allotrope with Massless Dirac Fermions. Physical Review Letters, 2014, 112, .	7.8	497
3	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
4	Structure prediction drives materials discovery. Nature Reviews Materials, 2019, 4, 331-348.	48.7	402
5	Unexpected Stable Stoichiometries of Sodium Chlorides. Science, 2013, 342, 1502-1505.	12.6	394
6	A stable compound of helium and sodium at high pressure. Nature Chemistry, 2017, 9, 440-445.	13.6	276
7	Rational design of all organic polymer dielectrics. Nature Communications, 2014, 5, 4845.	12.8	259
8	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
9	Predicting phase behavior of grain boundaries with evolutionary search and machine learning. Nature Communications, 2018, 9, 467.	12.8	122
10	Denser than diamond:Ab initiosearch for superdense carbon allotropes. Physical Review B, 2011, 83, .	3.2	118
11	Stability of xenon oxides at high pressures. Nature Chemistry, 2013, 5, 61-65.	13.6	118
12	Novel stable compounds in the Mgâ€“O system under high pressure. Physical Chemistry Chemical Physics, 2013, 15, 7696.	2.8	102
13	Evolutionary method for predicting surface reconstructions with variable stoichiometry. Physical Review B, 2013, 87, .	3.2	99
14	Computation and data driven discovery of topological phononic materials. Nature Communications, 2021, 12, 1204.	12.8	98
15	Powder diffraction and crystal structure prediction identify four new coumarin polymorphs. Chemical Science, 2017, 8, 4926-4940.	7.4	97
16	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 allotropes using evolutionary metadynamics. Physical Review B, 2012, 85, .	3.2	82
17	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
18	The Third Ambient Aspirin Polymorph. Crystal Growth and Design, 2017, 17, 3562-3566.	3.0	73

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19	Evolutionary metadynamics: a novel method to predict crystal structures. CrystEngComm, 2012, 14, 3596.	2.6	62
20	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
21	Grain boundary phases in bcc metals. Nanoscale, 2018, 10, 8253-8268.	5.6	55
22	ROY revisited, again: the eighth solved structure. Faraday Discussions, 2018, 211, 477-491.	3.2	55
23	Variable-composition structural optimization and experimental verification of MnB₃and MnB₄. Physical Chemistry Chemical Physics, 2014, 16, 15866-15873.	2.8	49
24	First-Principles Determination of the Structure of Magnesium Borohydride. Physical Review Letters, 2012, 109, 245503.	7.8	47
25	DDT Polymorphism and the Lethality of Crystal Forms. Angewandte Chemie - International Edition, 2017, 56, 10165-10169.	13.8	46
26	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
27	Computational Discovery of Inorganic Electrides from an Automated Screening. Matter, 2019, 1, 1293-1303.	10.0	42
28	Predicting polymeric crystal structures by evolutionary algorithms. Journal of Chemical Physics, 2014, 141, 154102.	3.0	41
29	PyXtal: A Python library for crystal structure generation and symmetry analysis. Computer Physics Communications, 2021, 261, 107810.	7.5	40
30	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
31	Pressure-induced structural and electronic transitions, metallization, and enhanced visible-light responsiveness in layered rhenium disulphide. Physical Review B, 2018, 97, .	3.2	35
32	Generalized evolutionary metadynamics for sampling the energy landscapes and its applications. Physical Review B, 2015, 92, .	3.2	33
33	Stable magnesium peroxide at high pressure. Scientific Reports, 2015, 5, 13582.	3.3	30
34	A Revisited Mechanism of the Graphite-to-Diamond Transition at High Temperature. Matter, 2020, 3, 864-878.	10.0	30
35	Predicting the ground-state structure of sodium boride. Physical Review B, 2018, 97, .	3.2	26
36	Ternary inorganic electrides with mixed bonding. Physical Review B, 2019, 99, .	3.2	26

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37	Magnetic borophenes from an evolutionary search. Physical Review B, 2019, 99, .	3.2	25
38	Tunable Contacts in Graphene/InSe van der Waals Heterostructures. Journal of Physical Chemistry C, 2020, 124, 23699-23706.	3.1	25
39	DDT Polymorphism and the Lethality of Crystal Forms. Angewandte Chemie, 2017, 129, 10299-10303.	2.0	21
40	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
41	Boron oxides under pressure: Prediction of the hardest oxides. Physical Review B, 2018, 98, .	3.2	18
42	Inverse Correlation between Lethality and Thermodynamic Stability of Contact Insecticide Polymorphs. Crystal Growth and Design, 2019, 19, 1839-1844.	3.0	18
43	PyXtal_FF: a python library for automated force field generation. Machine Learning: Science and Technology, 2021, 2, 027001.	5.0	18
44	Computational design of flexible electrides with nontrivial band topology. Physical Review Materials, 2019, 3, .	2.4	18
45	Electrides with Dinitrogen Ligands. ACS Applied Materials & Interfaces, 2019, 11, 5256-5263.	8.0	15
46	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
47	First-principles investigation of Sc-III/IV under high pressure. Physical Review B, 2018, 98, .	3.2	12
48	Neural network potential from bispectrum components: A case study on crystalline silicon. Journal of Chemical Physics, 2020, 153, 054118.	3.0	12
49	The stability and unexpected chemistry of oxide clusters. Physical Chemistry Chemical Physics, 2018, 20, 30437-30444.	2.8	11
50	Superconductivity in the van der Waals layered compound PS2. Physical Review B, 2019, 99, .	3.2	11
51	Structure-Controlled Oxygen Concentration in Fe₂O₃ and FeO₂. Inorganic Chemistry, 2019, 58, 5476-5482.	4.0	10
52	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
53	High dielectric ternary oxides from crystal structure prediction and high-throughput screening. Scientific Data, 2020, 7, 81.	5.3	9
54	Switchable two-dimensional electrides: A first-principles study. Physical Review B, 2021, 103, .	3.2	9

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55	Applications of crystal structure prediction â€“ organic molecular structures: general discussion. Faraday Discussions, 2018, 211, 493-539.	3.2	8
56	Crystal structure evaluation: calculating relative stabilities and other criteria: general discussion. Faraday Discussions, 2018, 211, 325-381.	3.2	7
57	Oligomer Hydrate Crystallization Improves Carbon Nanotube Memory. Chemistry of Materials, 2018, 30, 3813-3818.	6.7	6
58	Spectral neural network potentials for binary alloys. Journal of Applied Physics, 2020, 128, 045113.	2.5	4
59	Pressure-induced structural phase transition in Li4Ge. CrystEngComm, 2018, 20, 5949-5954.	2.6	2
60	Modeling surface spin polarization on ceria-supported Pt nanoparticles. Journal of Physics Condensed Matter, 2022, , .	1.8	0