Xin Zhao

List of Publications by Year in Descending Order

53 papers	877 citations	16 h-index	28 g-index
56 ext. papers	1,048 ext. citations	4.8 avg, IF	3.94 L-index

#	Paper	IF	Citations
53	Lithium nickel borides: evolution of [NiB] layers driven by Li pressure. *Inorganic Chemistry Frontiers*, **2021**, 8, 1675-1685	6.8	3
52	Stabilizing the crystal structures of NaFePO with Li substitutions. *Physical Chemistry Chemical Physics*, **2020**, 22, 13975-13980	3.6	2
51	Coherent band-edge oscillations and dynamic longitudinal-optical phonon mode splitting as evidence for polarons in perovskites. *Physical Review B*, **2020**, 101,	3.3	13
50	Theoretical search for possible LiNiB crystal structures using an adaptive genetic algorithm. *Journal of Applied Physics*, **2020**, 127, 094902	2.5	5
49	Light control of surface-bulk coupling by terahertz vibrational coherence in a topological insulator. *Npj Quantum Materials*, **2020**, 5,	5	23
48	Discovering rare-earth-free magnetic materials through the development of a database. *Physical Review Materials*, **2020**, 4,	3.2	2
47	Adaptive Genetic Algorithm for Structure Prediction and Application to Magnetic Materials **2020**, 2757-2776		
46	Ultrafast Control of Excitonic Rashba Fine Structure by Phonon Coherence in the Metal Halide Perovskite CH_{3}NH_{3}PbI_{3}. *Physical Review Letters*, **2020**, 124, 157401	7.4	16
45	Ultrafast nonthermal terahertz electrodynamics and possible quantum energy transfer in the Nb3Sn superconductor. *Physical Review B*, **2019**, 99,	3.3	15
44	Ultrafast manipulation of topologically enhanced surface transport driven by mid-infrared and terahertz pulses in BiSe. *Nature Communications*, **2019**, 10, 607	17.4	46
43	Computationally Driven Discovery of a Family of Layered LiNiB Polymorphs. *Angewandte Chemie*, **2019**, 131, 16002-16009	3.6	3
42	First-principles calculation of correlated electron materials based on Gutzwiller wave function beyond Gutzwiller approximation. *Journal of Physics Condensed Matter*, **2019**, 31, 335601	1.8	4
41	Computationally Driven Discovery of a Family of Layered LiNiB Polymorphs. *Angewandte Chemie - International Edition*, **2019**, 58, 15855-15862	16.4	13
40	Adaptive Genetic Algorithm for Structure Prediction and Application to Magnetic Materials **2019**, 1-20		
39	Correlation matrix renormalization theory for correlated-electron materials with application to the crystalline phases of atomic hydrogen. *Physical Review B*, **2018**, 97,	3.3	2
38	Ternary Bismuthide SrPtBi2: Computation and Experiment in Synergism to Explore Solid-State Materials. *Journal of Physical Chemistry C*, **2018**, 122, 5057-5063	3.8	2
37	New structures of Fe3S for rare-earth-free permanent magnets. *Journal Physics D: Applied Physics*, **2018**, 51, 075001	3	2

36	Fe-Si networks and charge/discharge-induced phase transitions in LiFeSiO cathode materials. *Physical Chemistry Chemical Physics*, **2018**, 20, 14557-14563	3.6	11
35	Spatially-correlated site occupancy in the nonstoichiometric meta-stable Al60Sm11 phase during devitrification of Al-10.2 at.% Sm glasses. *Acta Materialia*, **2018**, 156, 97-103	8.4	5
34	Structures and magnetic properties of iron silicide from adaptive genetic algorithm and first-principles calculations. *Journal of Applied Physics*, **2018**, 124, 073901	2.5	4
33	Magnetism of new metastable cobalt-nitride compounds. *Nanoscale*, **2018**, 10, 13011-13021	7.7	20
32	Influence of nitrogen dopants on the magnetization of Co3N clusters. *Physical Review Materials*, **2018**, 2,	3.2	5
31	Magnetocrystalline anisotropy in YCo5 and ZrCo5 compounds from first-principles real-space pseudopotentials calculations. *Physical Review Materials*, **2018**, 2,	3.2	3
30	Prediction of novel stable Fe-V-Si ternary phase. *Journal of Alloys and Compounds*, **2018**, 732, 567-572	5.7	2
29	An Efficient Scheme for Crystal Structure Prediction Based on Structural Motifs. *Journal of Physical Chemistry C*, **2017**, 121, 11891-11896	3.8	5
28	Exploring new phases of Fe3CoxC for rare-earth-free magnets. *Journal Physics D: Applied Physics*, **2017**, 50, 215005	3	6
27	Ultrafast terahertz snapshots of excitonic Rydberg states and electronic coherence in an organometal halide perovskite. *Nature Communications*, **2017**, 8, 15565	17.4	50
26	A scheme for the generation of FeP networks to search for low-energy LiFePO4 crystal structures. *Journal of Materials Chemistry A*, **2017**, 5, 14611-14618	13	9
25	Structures, phase transitions, and magnetic properties of Co3Si from first-principles calculations. *Physical Review B*, **2017**, 96,	3.3	6
24	Fe-Cluster Compounds of Chalcogenides: Candidates for Rare-Earth-Free Permanent Magnet and Magnetic Nodal-Line Topological Material. *Inorganic Chemistry*, **2017**, 56, 14577-14583	5.1	3
23	Theoretical search for possible Au-Si crystal structures using a genetic algorithm. *Physical Review B*, **2017**, 95,	3.3	7
22	Metastable cobalt nitride structures with high magnetic anisotropy for rare-earth free magnets. *Physical Chemistry Chemical Physics*, **2016**, 18, 31680-31690	3.6	23
21	Zero-Strain Na2FeSiO4 as Novel Cathode Material for Sodium-Ion Batteries. *ACS Applied Materials & Interfaces*, **2016**, 8, 17233-8	9.5	80
20	Large magnetic anisotropy predicted for rare-earth-free Fe16CoxN2 alloys. *Physical Review B*, **2016**, 94,	3.3	31
19	Robust diamond-like Fe-Si network in the zero-strain Na FeSiO4 cathode. *Electrochimica Acta*, **2016**, 212, 934-940	6.7	27

18	Fe-Si networks in Na2FeSiO4 cathode materials. *Physical Chemistry Chemical Physics*, **2016**, 18, 23916-22	3.6	23
17	Cluster expansion modeling and Monte Carlo simulation of alnico 5 permanent magnets. *Journal of Applied Physics*, **2015**, 117, 093905	2.5	5
16	Electronic structure of Ce2RhIn8: A two-dimensional heavy-fermion system studied by angle-resolved photoemission spectroscopy. *Physical Review B*, **2015**, 91,	3.3	9
15	Exploration of tetrahedral structures in silicate cathodes using a motif-network scheme. *Scientific Reports*, **2015**, 5, 15555	4.9	24
14	Structures and magnetic properties of Co-Zr-B magnets studied by first-principles calculations. *Journal of Applied Physics*, **2015**, 117, 243902	2.5	12
13	First-principles study of direct and narrow band gap semiconductingCuGaO2. *Materials Research Express*, **2015**, 2, 045902	1.7	9
12	Orthorhombic Zr2Co11 phase revisited. *Journal of Alloys and Compounds*, **2014**, 611, 167-170	5.7	5
11	sp3-hybridized framework structure of group-14 elements discovered by genetic algorithm. *Physical Review B*, **2014**, 89,	3.3	20
10	An adaptive genetic algorithm for crystal structure prediction. *Journal of Physics Condensed Matter*, **2014**, 26, 035402	1.8	75
9	New Be-intercalated hexagonal boron layer structure of BeB2. *RSC Advances*, **2014**, 4, 15061-15065	3.7	2
8	Interface Structure Prediction from First-Principles. *Journal of Physical Chemistry C*, **2014**, 118, 9524-9530	3.8	28
7	Exploring the structural complexity of intermetallic compounds by an adaptive genetic algorithm. *Physical Review Letters*, **2014**, 112, 045502	7.4	78
6	New stable Re-B phases for ultra-hard materials. *Journal of Physics Condensed Matter*, **2014**, 26, 455401	1.8	5
5	Genetic algorithm prediction of crystal structure of metastable Si-IX phase. *Solid State Communications*, **2014**, 182, 14-16	1.6	6
4	New layered structures of cuprous chalcogenides as thin film solar cell materials: Cu2Te and Cu2Se. *Physical Review Letters*, **2013**, 111, 165502	7.4	88
3	Atomic Structure and Magnetic Properties of HfCo$_{7}$ Alloy. *IEEE Transactions on Magnetics*, **2013**, 49, 3281-3283	2	6
2	Structures and stabilities of alkaline earth metal peroxides XO2 (X = Ca, Be, Mg) studied by a genetic algorithm. *RSC Advances*, **2013**, 3, 22135	3.7	16
1	Atomic structure and magnetic properties of Fe1Cox alloys. *Journal of Applied Physics*, **2012**, 111, 07E338	2.5	18