## Chao Zhang

List of Publications by Year in descending order

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331259 476904 1,005 68 21 29 h-index citations g-index papers 68 68 68 1204 docs citations times ranked citing authors all docs

#	Article	IF	CITATIONS
1	Enhancement of the thermoelectric performance of bulk SnTe alloys via the synergistic effect of band structure modification and chemical bond softening. Journal of Materials Chemistry A, 2017, 5, 14165-14173.	5.2	65
2	Structural, Electronic, Dynamical, and Superconducting Properties in Dense GeH <sub>4</sub> (H <sub>2</sub> ) <sub>2</sub> . Journal of Physical Chemistry C, 2012, 116, 5225-5234.	1.5	55
3	Strain Induced Band Dispersion Engineering in Si Nanosheets. Journal of Physical Chemistry C, 2011, 115, 23682-23687.	1.5	54
4	Substitutional position and insulator-to-metal transition in Nb-doped SrTiO3. Materials Chemistry and Physics, 2008, 107, 215-219.	2.0	48
5	Structural and electronic properties of Fe-doped BaTiO 3 and SrTiO 3. Chinese Physics B, 2007, 16, 1422-1428.	1.3	40
6	Development of a deep machine learning interatomic potential for metalloid-containing Pd-Si compounds. Physical Review B, 2019, 100, .	1.1	39
7	<mml:math <br="" xmlns:mml="http://www.w3.org/1998/Math/MathML">display="inline"&gt;<mml:mi>\i^2</mml:mi><mml:mtext mathvariant="normal"&gt;\hata^'<mml:mi>tin</mml:mi><mml:mo>\hata†'</mml:mo><mml:mi>I</mml:mi><i Transitions of Germanium, Physical Review Letters, 2011, 106, 135502.</i </mml:mtext </mml:math>	mmी:mi>n	n <m< td=""></m<>
8	Constraint on the potassium content for the superconductivity of potassium-intercalated phenanthrene. Journal of Chemical Physics, 2014, 140, 114301.	1.2	36
9	Structural and Bonding Characteristics of Potassium-Doped <i>p</i> -Terphenyl Superconductors. Journal of Physical Chemistry C, 2018, 122, 3801-3808.	1.5	36
10	Phase transformations and vibrational properties of coronene under pressure. Journal of Chemical Physics, 2013, 139, 144308.	1.2	35
11	Pressure-induced superconductivity in H2-containing hydride PbH4(H2)2. Scientific Reports, 2015, 5, 16475.	1.6	35
12	Superconductivity and phase stability of potassium-doped biphenyl. Physical Chemistry Chemical Physics, 2018, 20, 25217-25223.	1.3	31
13	Topochemical Deintercalation of Li from Layered LiNiB: toward 2D MBene. Journal of the American Chemical Society, 2021, 143, 4213-4223.	6.6	28
14	High thermopower and potential thermoelectric properties of crystalline LiH and NaH. Physical Review B, 2017, 95, .	1.1	26
15	A deep learning interatomic potential developed for atomistic simulation of carbon materials. Carbon, 2022, 186, 1-8.	5.4	25
16	Magnetic instability and pair binding in aromatic hydrocarbon superconductors. Scientific Reports, 2012, 2, 922.	1.6	24
17	Structural and vibrational properties of phenanthrene under pressure. Journal of Chemical Physics, 2013, 139, 104302.	1.2	24
18	Intrinsic electronic transport and thermoelectric power factor in n-type doped monolayer MoS <sub>2</sub> . New Journal of Physics, 2018, 20, 043009.	1.2	23

#	Article	IF	Citations
19	Cage Structure and Near Room-Temperature Superconductivity in TbH <i><sub>n</sub></i> ( <i>n</i> =) Tj ETQq1	1.9.7843	14 rgBT /0
20	Superconductivity in Hydrogen-rich Material: GeH4. Journal of Superconductivity and Novel Magnetism, 2010, 23, 717-719.	0.8	22
21	Structural transitions of solid germane under pressure. Europhysics Letters, 2010, 90, 66006.	0.7	22
22	Chemical Trend of Pressure-Induced Metallization in Alkaline Earth Hydrides. Journal of Physical Chemistry C, 2010, 114, 14614-14617.	1.5	20
23	Structural and electronic properties of potassium-doped 1,2;8,9-dibenzopentacene superconductor: comparing with doped [7]phenacenes. Molecular Physics, 2017, 115, 472-483.	0.8	18
24	First-principles investigations on the magnetic property in tripotassium doped picene. Journal of Applied Physics, 2013, 113, 17E131.	1.1	14
25	Phase transitions and electron–phonon coupling in platinum hydride. Journal of Physics Condensed Matter, 2012, 24, 035701.	0.7	12
26	Structural and polarization properties of short-periodSrZrO3â^•SrTiO3superlattices. Physical Review B, 2007, 75, .	1.1	11
27	Superconductivity in GeH4(H2)2 above 220GPa high-pressure. Physica B: Condensed Matter, 2013, 410, 90-92.	1.3	11
28	Stable and Metastable Structures in Compressed LiC <sub>6</sub> : Dimensional Diversity. Journal of Physical Chemistry C, 2016, 120, 10137-10145.	1.5	11
29	Coincidence angle-resolved photoemission spectroscopy: Proposal for detection of two-particle correlations. Physical Review B, 2020, 101, .	1.1	11
30	Discovering rare-earth-free magnetic materials through the development of a database. Physical Review Materials, 2020, 4, .	0.9	11
31	Dopant position in Ti-doped high-temperature phase Ta2O5: First principles study. Applied Physics Letters, 2007, 91, .	1.5	9
32	Mechanical and thermodynamic properties of α-UH3 under pressure. Journal of Alloys and Compounds, 2014, 604, 171-174.	2.8	9
33	Stabilizing and activating dopants in âŸ˙112⟩ silicon nanowires by alkene adsorptions: A first-principles study. Applied Physics Letters, 2011, 98, 073115.	1.5	8
34	Phonon-mediated superconductivity in quasi-1D Sc <sub>3</sub> CoC <sub>4</sub> . Europhysics Letters, 2012, 100, 67003.	0.7	8
35	Vibrational and structural properties of tetramethyltin under pressure. Journal of Chemical Physics, 2013, 138, 024307.	1.2	8
36	Pressure-Induced Novel Stable Stoichiometries in Molybdenum–Phosphorus Phase Diagrams under Pressure. Journal of Physical Chemistry C, 2019, 123, 30187-30197.	1.5	8

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37	Deep machine learning potential for atomistic simulation of Fe-Si-O systems under Earth's outer core conditions. Physical Review Materials, 2022, 6, .	0.9	8
38	High-pressure phases of a hydrogen-rich compound: Tetramethylgermane. Physical Review B, 2012, 86, .	1.1	7
39	Phase transitions of actinium dihydride: Pressure-induced charge transfer driving effect. International Journal of Hydrogen Energy, 2014, 39, 15827-15835.	3.8	7
40	Zero-Point Effects on Phase Transitions of Thorium Dihydride under High Pressure. Journal of Physical Chemistry C, 2015, 119, 13465-13471.	1.5	7
41	Crystallization of the P <sub>3</sub> Sn <sub>4</sub> Phase upon Cooling P <sub>2</sub> Sn <sub>5</sub> Liquid by Molecular Dynamics Simulation Using a Machine Learning Interatomic Potential. Journal of Physical Chemistry C, 2021, 125, 3127-3133.	1.5	7
42	Inducing novel electronic properties in âŒ@112〉 Ge nanowires by means of variations in their size, shape and strain: a first-principles computational study. Journal of Physics Condensed Matter, 2012, 24, 015301.	0.7	6
43	Electrical and luminescence properties, and energy band structure of SrBi2-Er Nb2O9 multifunctional ceramics. Ceramics International, 2021, 47, 30938-30946.	2.3	6
44	Neural network potential for Zr–Rh system by machine learning. Journal of Physics Condensed Matter, 2022, 34, 075402.	0.7	6
45	Effect of carbon content and electronic strong correlation on the mechanical and thermodynamic properties of ytterbium carbides. RSC Advances, 2015, 5, 103082-103090.	1.7	5
46	Mechanical anisotropy and ideal strength of ThBC. Journal of Physics and Chemistry of Solids, 2018, 122, 203-209.	1.9	5
47	Straintronic Effect on Phonon-Mediated Superconductivity of Nb <sub>2</sub> CT <sub>2</sub> (T = O,) Tj ETQq1	1.0.7843 1.5	14 rgBT /0
48	Sm-modified bismuth layer-structured SrBi2Nb2O9 multifunctional ceramics with enhanced electrical properties and good photoluminescence properties. Ceramics International, 2022, 48, 18989-18998.	2.3	5
49	Pb-driven anti-ferroelectric phase in Pb(Mg1/3Nb2/3)O3 : First-principle study. Solid State Communications, 2008, 145, 299-302.	0.9	3
50	Spin polarization of polaron in quasi-one dimensional organic system. Modern Physics Letters B, 2015, 29, 1450266.	1.0	3
51	Influence of orbital nematic order on spin responses in Fe-based superconductors. Physics Letters, Section A: General, Atomic and Solid State Physics, 2016, 380, 2008-2012.	0.9	3
52	Spin Excitation Under Electron Delocalization of Side Radicals in Quasi-One-Dimensional Organic Ferromagnet. Journal of Electronic Materials, 2017, 46, 1005-1009.	1.0	3
53	Magnetic Transitions in K-Doped Biphenyl and $p$ -Terphenyl. IEEE Transactions on Magnetics, 2018, 54, 1-5.	1.2	3
54	Predicting magnetic anisotropy energies using site-specific spin-orbit coupling energies and machine learning: Application to iron-cobalt nitrides. Physical Review Materials, 2022, 6, .	0.9	3

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55	Surface rumples and band gap reductions of cubic BaZrO <sub>3</sub> (001) surface studied by means of first-principles calculations. Chinese Physics B, 2008, 17, 274-280.	0.7	2
56	Thermodynamic and mechanical properties of actinium and lanthanum dihydride. Journal of Alloys and Compounds, 2014, 616, 42-46.	2.8	2
57	Pressure dependent mechanical properties of calcium carbides. Ceramics International, 2018, 44, 7429-7434.	2.3	2
58	Robust quantum spin Hall state and quantum anomalous Hall state in graphenelike BC3 with adatoms. New Journal of Physics, 2018, 20, 073047.	1.2	2
59	An ultra-incompressible Mn3N compound predicted by first-principles genetic algorithm. Journal of Applied Physics, 2020, 128, 055112.	1.1	2
60	Hydrogenation as a source of superconductivity in two-dimensional TiB2. International Journal of Modern Physics C, 2021, 32, 2150057.	0.8	2
61	Photoluminescence, electrical properties and electron band structure of (Ho, Yb)3+ co-doped SrBi4Ti4O15 multifunctional ceramics. Ceramics International, 2022, 48, 9248-9257.	2.3	2
62	Strong correlation effect on the thermodynamic and mechanical properties of ytterbium dihydride. International Journal of Hydrogen Energy, 2016, 41, 21286-21292.	3.8	1
63	Superconductivity in $\hat{I}^2$ -Tin Germanium. Journal of Superconductivity and Novel Magnetism, 2013, 26, 2009-2011.	0.8	0
64	Superconductivity driven by pairing of the coherent parts of the physical electrons. Physica C: Superconductivity and Its Applications, 2018, 546, 21-27.	0.6	0
65	The Zeno effect and relaxation rates in a triple quantum dot system. European Physical Journal B, 2018, 91, 1.	0.6	0
66	Coincidence inelastic neutron scattering for detection of two-spin magnetic correlations. Physical Review B, 2021, 103, .	1.1	0
67	Chemical physics of superconductivity in layered yttrium carbide halides from first principles. Physical Review B, 2021, 103, .	1.1	0
68	Phase transition and enhanced hardness of LaB4 under pressure. Journal of Physics and Chemistry of Solids, 2022, , 110622.	1.9	0