

Chao Zhang

List of Publications by Year in descending order

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331259

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68
all docs

68
docs citations

68
times ranked

1204
citing authors

#	ARTICLE	IF	CITATIONS
1	A deep learning interatomic potential developed for atomistic simulation of carbon materials. Carbon, 2022, 186, 1-8.	5.4	25
2	Neural network potential for Zr-Rh system by machine learning. Journal of Physics Condensed Matter, 2022, 34, 075402.	0.7	6
3	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
4	Straintronic Effect on Phonon-Mediated Superconductivity of Nb ₂ CT ₂ (T = O,) Tj ETQq0 0.0 rgBT / Overlock 10	1.5	5
5	Phase transition and enhanced hardness of LaB ₄ under pressure. Journal of Physics and Chemistry of Solids, 2022, , 110622.	1.9	0
6	Sm-modified bismuth layer-structured SrBi ₂ Nb ₂ O ₉ multifunctional ceramics with enhanced electrical properties and good photoluminescence properties. Ceramics International, 2022, 48, 18989-18998.	2.3	5
7	Photoluminescence, electrical properties and electron band structure of (Ho, Yb) ³⁺ co-doped SrBi ₄ Ti ₄ O ₁₅ multifunctional ceramics. Ceramics International, 2022, 48, 9248-9257.	2.3	2
8	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
9	Crystallization of the P ₃ Sn ₄ Phase upon Cooling P ₂ Sn ₅ Liquid by Molecular Dynamics Simulation Using a Machine Learning Interatomic Potential. Journal of Physical Chemistry C, 2021, 125, 3127-3133.	1.5	7
10	Hydrogenation as a source of superconductivity in two-dimensional TiB ₂ . International Journal of Modern Physics C, 2021, 32, 2150057.	0.8	2
11	Cage Structure and Near Room-Temperature Superconductivity in TbH _n (<i>n</i> =) Tj ETQq1 1.0.784314 rgBT / Cw	1.5	23
12	Coincidence inelastic neutron scattering for detection of two-spin magnetic correlations. Physical Review B, 2021, 103, .	1.1	0
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	Chemical physics of superconductivity in layered yttrium carbide halides from first principles. Physical Review B, 2021, 103, .	1.1	0
15	Electrical and luminescence properties, and energy band structure of SrBi ₂ -Er Nb ₂ O ₉ multifunctional ceramics. Ceramics International, 2021, 47, 30938-30946.	2.3	6
16	An ultra-incompressible Mn ₃ N compound predicted by first-principles genetic algorithm. Journal of Applied Physics, 2020, 128, 055112.	1.1	2
17	Coincidence angle-resolved photoemission spectroscopy: Proposal for detection of two-particle correlations. Physical Review B, 2020, 101, .	1.1	11
18	Discovering rare-earth-free magnetic materials through the development of a database. Physical Review Materials, 2020, 4, .	0.9	11

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19	Development of a deep machine learning interatomic potential for metalloids-containing Pd-Si compounds. <i>Physical Review B</i> , 2019, 100, .	1.1	39
20	Pressure-Induced Novel Stable Stoichiometries in Molybdenum-Phosphorus Phase Diagrams under Pressure. <i>Journal of Physical Chemistry C</i> , 2019, 123, 30187-30197.	1.5	8
21	Intrinsic electronic transport and thermoelectric power factor in n-type doped monolayer MoS ₂ . <i>New Journal of Physics</i> , 2018, 20, 043009.	1.2	23
22	Structural and Bonding Characteristics of Potassium-Doped <i>p</i> -Terphenyl Superconductors. <i>Journal of Physical Chemistry C</i> , 2018, 122, 3801-3808.	1.5	36
23	Pressure dependent mechanical properties of calcium carbides. <i>Ceramics International</i> , 2018, 44, 7429-7434.	2.3	2
24	Superconductivity driven by pairing of the coherent parts of the physical electrons. <i>Physica C: Superconductivity and Its Applications</i> , 2018, 546, 21-27.	0.6	0
25	The Zeno effect and relaxation rates in a triple quantum dot system. <i>European Physical Journal B</i> , 2018, 91, 1.	0.6	0
26	Superconductivity and phase stability of potassium-doped biphenyl. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 25217-25223.	1.3	31
27	Mechanical anisotropy and ideal strength of ThBC. <i>Journal of Physics and Chemistry of Solids</i> , 2018, 122, 203-209.	1.9	5
28	Robust quantum spin Hall state and quantum anomalous Hall state in graphenelike BC3 with adatoms. <i>New Journal of Physics</i> , 2018, 20, 073047.	1.2	2
29	Magnetic Transitions in K-Doped Biphenyl and <i>p</i> -Terphenyl. <i>IEEE Transactions on Magnetics</i> , 2018, 54, 1-5.	1.2	3
30	Structural and electronic properties of potassium-doped 1,2;8,9-dibenzopentacene superconductor: comparing with doped [7]phenacenes. <i>Molecular Physics</i> , 2017, 115, 472-483.	0.8	18
31	Spin Excitation Under Electron Delocalization of Side Radicals in Quasi-One-Dimensional Organic Ferromagnet. <i>Journal of Electronic Materials</i> , 2017, 46, 1005-1009.	1.0	3
32	High thermopower and potential thermoelectric properties of crystalline LiH and NaH. <i>Physical Review B</i> , 2017, 95, .	1.1	26
33	Enhancement of the thermoelectric performance of bulk SnTe alloys via the synergistic effect of band structure modification and chemical bond softening. <i>Journal of Materials Chemistry A</i> , 2017, 5, 14165-14173.	5.2	65
34	Influence of orbital nematic order on spin responses in Fe-based superconductors. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2016, 380, 2008-2012.	0.9	3
35	Stable and Metastable Structures in Compressed LiC ₆ : Dimensional Diversity. <i>Journal of Physical Chemistry C</i> , 2016, 120, 10137-10145.	1.5	11
36	Strong correlation effect on the thermodynamic and mechanical properties of ytterbium dihydride. <i>International Journal of Hydrogen Energy</i> , 2016, 41, 21286-21292.	3.8	1

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37	Pressure-induced superconductivity in H ₂ -containing hydride PbH ₄ (H ₂) ₂ . Scientific Reports, 2015, 5, 16475.	1.6	35
38	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
39	Spin polarization of polaron in quasi-one dimensional organic system. Modern Physics Letters B, 2015, 29, 1450266.	1.0	3
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	Mechanical and thermodynamic properties of $\hat{I}\pm$ -UH ₃ under pressure. Journal of Alloys and Compounds, 2014, 604, 171-174.	2.8	9
42	Constraint on the potassium content for the superconductivity of potassium-intercalated phenanthrene. Journal of Chemical Physics, 2014, 140, 114301.	1.2	36
43	Phase transitions of actinium dihydride: Pressure-induced charge transfer driving effect. International Journal of Hydrogen Energy, 2014, 39, 15827-15835.	3.8	7
44	Thermodynamic and mechanical properties of actinium and lanthanum dihydride. Journal of Alloys and Compounds, 2014, 616, 42-46.	2.8	2
45	Superconductivity in \hat{I}^2 -Tin Germanium. Journal of Superconductivity and Novel Magnetism, 2013, 26, 2009-2011.	0.8	0
46	Structural and vibrational properties of phenanthrene under pressure. Journal of Chemical Physics, 2013, 139, 104302.	1.2	24
47	Superconductivity in GeH ₄ (H ₂) ₂ above 220GPa high-pressure. Physica B: Condensed Matter, 2013, 410, 90-92.	1.3	11
48	Vibrational and structural properties of tetramethyltin under pressure. Journal of Chemical Physics, 2013, 138, 024307.	1.2	8
49	First-principles investigations on the magnetic property in tripotassium doped picene. Journal of Applied Physics, 2013, 113, 17E131.	1.1	14
50	Phase transformations and vibrational properties of coronene under pressure. Journal of Chemical Physics, 2013, 139, 144308.	1.2	35
51	Magnetic instability and pair binding in aromatic hydrocarbon superconductors. Scientific Reports, 2012, 2, 922.	1.6	24
52	Inducing novel electronic properties in $\hat{C}\text{e}^{112}\hat{C}\text{e}^3$ 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
53	High-pressure phases of a hydrogen-rich compound: Tetramethylgermane. Physical Review B, 2012, 86, .	1.1	7
54	Phase transitions and electron-phonon coupling in platinum hydride. Journal of Physics Condensed Matter, 2012, 24, 035701.	0.7	12

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55	Structural, Electronic, Dynamical, and Superconducting Properties in Dense GeH ₄ (H ₂) ₂ . Journal of Physical Chemistry C, 2012, 116, 5225-5234.	1.5	55
56	Phonon-mediated superconductivity in quasi-1D Sc ₃ CoC ₄ . Europhysics Letters, 2012, 100, 67003.	0.7	8
57	Strain Induced Band Dispersion Engineering in Si Nanosheets. Journal of Physical Chemistry C, 2011, 115, 23682-23687.	1.5	54
58	$\langle \text{mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"} \rangle \langle \text{mml:mi} \rangle \hat{I}^2 \langle \text{mml:mi} \rangle \langle \text{mml:mtext mathvariant="normal"} \rangle \hat{a}^{\prime} \langle \text{mml:mtext} \rangle \langle \text{mml:mi} \rangle \text{tin} \langle \text{mml:mi} \rangle \langle \text{mml:mo} \rangle \hat{a}^{\dagger} \langle \text{mml:mo} \rangle \langle \text{mml:mi} \rangle \text{I} \langle \text{mml:mi} \rangle \langle \text{mml:mi} \rangle \text{m} \langle \text{mml:mi} \rangle \text{m}$ Transitions of Germanium. Physical Review Letters, 2011, 106, 135502.	2.9	38
59	Stabilizing and activating dopants in $\hat{Y}^{112}\hat{Y}^{\text{C}}$ silicon nanowires by alkene adsorptions: A first-principles study. Applied Physics Letters, 2011, 98, 073115.	1.5	8
60	Superconductivity in Hydrogen-rich Material: GeH ₄ . Journal of Superconductivity and Novel Magnetism, 2010, 23, 717-719.	0.8	22
61	Structural transitions of solid germane under pressure. Europhysics Letters, 2010, 90, 66006.	0.7	22
62	Chemical Trend of Pressure-Induced Metallization in Alkaline Earth Hydrides. Journal of Physical Chemistry C, 2010, 114, 14614-14617.	1.5	20
63	Pb-driven anti-ferroelectric phase in Pb(Mg _{1/3} Nb _{2/3})O ₃ : First-principle study. Solid State Communications, 2008, 145, 299-302.	0.9	3
64	Substitutional position and insulator-to-metal transition in Nb-doped SrTiO ₃ . Materials Chemistry and Physics, 2008, 107, 215-219.	2.0	48
65	Surface rumples and band gap reductions of cubic BaZrO ₃ (001) surface studied by means of first-principles calculations. Chinese Physics B, 2008, 17, 274-280.	0.7	2
66	Structural and polarization properties of short-period SrZrO ₃ \hat{a} •SrTiO ₃ superlattices. Physical Review B, 2007, 75, .	1.1	11
67	Structural and electronic properties of Fe-doped BaTiO ₃ and SrTiO ₃ . Chinese Physics B, 2007, 16, 1422-1428.	1.3	40
68	Dopant position in Ti-doped high-temperature phase Ta ₂ O ₅ : First principles study. Applied Physics Letters, 2007, 91, .	1.5	9