Yansun Yao

List of Publications by Year in descending order

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91 papers	2,166 citations	236925 25 h-index	265206 42 g-index
91 all docs	91 docs citations	91 times ranked	1939 citing authors

#	Article	IF	Citations
1	Design Principles for High-Temperature Superconductors with a Hydrogen-Based Alloy Backbone at Moderate Pressure. Physical Review Letters, 2022, 128, 047001.	7.8	91
2	Elucidating the reaction pathway of crystalline multi-metal borides for highly efficient oxygen-evolving electrocatalysts. Journal of Materials Chemistry A, 2022, 10, 1569-1578.	10.3	13
3	Path to high- <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>T</mml:mi><mml:mi mathvariant="normal">c</mml:mi></mml:msub></mml:math> superconductivity via Rb substitution of guest metal atoms in the <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Sr</mml:mi><mml:msub><mml:mi mathvariant="normal">B</mml:mi><mml:mn>3</mml:mn></mml:msub><mml:msub><mml:mi mathvariant	3.2	17
4	Dirac nodal-line semimetal zinc polynitride at high pressure. Physical Review B, 2022, 105, .	3.2	2
5	Theoretical methods for structural phase transitions in elemental solids at extreme conditions: statics and dynamics. Journal of Physics Condensed Matter, 2022, 34, 363001.	1.8	1
6	Structural diversity and unusual valence states in compressed Na-Hg system. Computational Materials Science, 2022, 211, 111561.	3.0	0
7	High-pressure structural study of Î± -Mn: Experiments and calculations. Physical Review B, 2021, 103, .	3.2	1
8	Machine learning metadynamics simulation of reconstructive phase transition. Physical Review B, 2021, 103, .	3.2	15
9	IrN4 and IrN7 as potential high-energy-density materials. Journal of Chemical Physics, 2021, 154, 054706.	3.0	11
10	Quantum and Classical Proton Diffusion in Superconducting Clathrate Hydrides. Physical Review Letters, 2021, 126, 117002.	7.8	17
11	Synthesis of superconducting SbS and SbS2 antimony chalcogenide compounds at high pressures. Physical Review B, 2021, 103, .	3.2	2
12	Solid Nitrogen and Nitrogenâ€Rich Compounds as Highâ€Energyâ€Density Materials. Physica Status Solidi (B): Basic Research, 2021, 258, 2000588.	1.5	12
13	Potassium-activated anionic copper and covalent Cuâ€“Cu bonding in compressed Kâ€“Cu compounds. Journal of Chemical Physics, 2021, 154, 134708.	3.0	5
14	Prediction of a stable helium-hydrogen compound: First-principles simulations. Physical Review B, 2021, 104, .	3.2	4
15	First-principles investigation of rhodium hydrides under high pressure. Physical Review B, 2021, 104, .	3.2	4
16	Oxysulfide Li2BeSO: A potential new material for solid electrolyte predicted from first principles. Journal of Alloys and Compounds, 2020, 818, 152844.	5.5	1
17	Superconducting Zirconium Polyhydrides at Moderate Pressures. Journal of Physical Chemistry Letters, 2020, 11, 646-651.	4.6	26
18	Hydrogen Pentagraphenelike Structure Stabilized by Hafnium: A High-Temperature Conventional Superconductor. Physical Review Letters, 2020, 125, 217001.	7.8	87

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19	Two good metals make a semiconductor: A potassium-nickel compound under pressure. Physical Review B, 2020, 102, .	3.2	7
20	o-C240: a new sp3-dominated allotrope of carbon. Journal of Physics Condensed Matter, 2020, 32, 395401.	1.8	12
21	Formation of Stable Compounds of Potassium and Iron under Pressure. Journal of Physical Chemistry A, 2020, 124, 4752-4763.	2.5	6
22	Nitrogen in black phosphorus structure. Science Advances, 2020, 6, eaba9206.	10.3	90
23	Pressure-induced structural transformations and new polymorphs in BiVO₄. Physical Chemistry Chemical Physics, 2020, 22, 10238-10246.	2.8	9
24	Pressure-induced decomposition of binary lanthanum intermetallic compounds. Physical Review B, 2020, 101, .	3.2	9
25	High-enthalpy crystalline phases of cadmium telluride. Physical Review Research, 2020, 2, .	3.6	4
26	A High-Pressure Compound of Argon and Nickel: Noble Gas in the Earthâ€™s Core?. ACS Earth and Space Chemistry, 2019, 3, 2517-2524.	2.7	10
27	High-temperature shape memory loss in nitinol: a first principles study. Physical Chemistry Chemical Physics, 2019, 21, 7508-7517.	2.8	7
28	Mechanism for the Structural Transformation to the Modulated Superconducting Phase of Compressed Hydrogen Sulfide. Scientific Reports, 2019, 9, 5023.	3.3	12
29	Synthesis of Xenon and Iron-Nickel Intermetallic Compounds at Earthâ€™s Core Thermodynamic Conditions. Physical Review Letters, 2018, 120, 096001.	7.8	39
30	Frontispiece: Superconducting Hydrogen Sulfide. Chemistry - A European Journal, 2018, 24, .	3.3	0
31	B1-B2 phase transition mechanism and pathway of PbS under pressure. Journal of Chemical Physics, 2018, 148, 104503.	3.0	7
32	Revealing the formation mechanism of ultrahard nanotwinned diamond from onion carbon. Carbon, 2018, 129, 159-167.	10.3	40
33	Superconducting Hydrogen Sulfide. Chemistry - A European Journal, 2018, 24, 1769-1778.	3.3	32
34	Crystal structures of transition metal pernitrides predicted from first principles. RSC Advances, 2018, 8, 36412-36421.	3.6	15
35	Prediction of Stable Iron Nitrides at Ambient and High Pressures with Progressive Formation of New Polynitrogen Species. Chemistry of Materials, 2018, 30, 8476-8485.	6.7	56
36	Using coherent phonons for ultrafast control of the Dirac node of SrMnSb2. Physical Review B, 2018, 98, .	3.2	14

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37	Reply to Datchi et al.: Recovered phase CO2-V at low temperature and a newly predicted 3D-extended CO2phase. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, E658-E659.	7.1	1
38	Piezochromism and structural and electronic properties of benz[a]anthracene under pressure. Physical Chemistry Chemical Physics, 2017, 19, 6216-6223.	2.8	19
39	Pressure-Induced Polymorphic, Optical, and Electronic Transitions of Formamidinium Lead Iodide Perovskite. Journal of Physical Chemistry Letters, 2017, 8, 2119-2125.	4.6	115
40	Novel boron channel-based structure of boron carbide at high pressures. Journal of Physics Condensed Matter, 2017, 29, 455401.	1.8	1
41	Modulated Structure Calculated for Superconducting Hydrogen Sulfide. Angewandte Chemie, 2017, 129, 11548-11551.	2.0	4
42	Modulated Structure Calculated for Superconducting Hydrogen Sulfide. Angewandte Chemie - International Edition, 2017, 56, 11390-11393.	13.8	21
43	New multifunctional tungsten nitride with energetic N ₆ and extreme hardness predicted from first principles. Europhysics Letters, 2017, 118, 46001.	2.0	23
44	High-pressure phase transition of alkali metalâ€“transition metal deuteride Li2PdD2. Journal of Chemical Physics, 2017, 146, 234506.	3.0	2
45	Superconductivity in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>FeH</mml:mi><mml:mn>5</mml:mn></mml:msub></m Physical Review B, 2017, 96, .	3.2	45
46	Stable BaCl solid at high pressure: Prediction and characterization using first principles approach. Journal of Applied Physics, 2017, 122, 235902.	2.5	2
47	Single-bonded allotrope of nitrogen predicted at high pressure. Physical Review B, 2017, 96, .	3.2	36
48	High-pressure X-ray diffraction, Raman and computational studies of MgCl2 up to 1 Mbar: Extensive pressure stability of the Î²-MgCl2 layered structure. Scientific Reports, 2016, 6, 30631.	3.3	15
49	High pressure structural changes in aluminium triiodide: A first principles study. Journal of Chemical Physics, 2016, 144, 124507.	3.0	2
50	A New Allotrope of Nitrogen as High-Energy Density Material. Journal of Physical Chemistry A, 2016, 120, 2920-2925.	2.5	73
51	Pressure-driven suppression of the Jahnâ€“Teller effects and structural changes in cupric oxide. Journal of Physics Condensed Matter, 2016, 28, 025401.	1.8	7
52	Crystal structures and dynamical properties of dense CO ₂. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 11110-11115.	7.1	28
53	High-pressure structural study of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>MnF</mml:mi><mml:mn>2</mml:mn></mml:msub></m Physical Review B, 2016, 93, .	3.2	26
54	Prediction of a stable half-metal ferromagnetic BaCl solid. Physical Review B, 2016, 93, .	3.2	6

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55	Stable Calcium Nitrides at Ambient and High Pressures. Inorganic Chemistry, 2016, 55, 7550-7555.	4.0	88
56	Coexistence of Superconductivity and Superhardness in Beryllium Hexaboride Driven by Inherent Multicenter Bonding. Journal of Physical Chemistry Letters, 2016, 7, 4898-4904.	4.6	16
57	Structures of Nanoalloy Clusters Au_nAl_n (n = 1â€“10) and the Growth Patterns to the Bulk Phase. Journal of Physical Chemistry C, 2016, 120, 25588-25595.	3.1	9
58	Hydrogen segregation and its roles in structural stability and metallization: silane under pressure. Scientific Reports, 2015, 5, 13039.	3.3	17
59	Exotic stable cesium polynitrides at high pressure. Scientific Reports, 2015, 5, 16902.	3.3	58
60	Theoretical Predictions of Novel Superconducting Phases of BaGe3 Stable at Atmospheric and High Pressures. Inorganic Chemistry, 2015, 54, 2875-2884.	4.0	17
61	Crystalline LiN₅ Predicted from First-Principles as a Possible High-Energy Material. Journal of Physical Chemistry Letters, 2015, 6, 2363-2366.	4.6	145
62	Stable structures of He and<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi mathvariant="normal">H</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mi mathvariant="normal">O</mml:mi></mml:mrow></mml:math>at high pressure. Physical Review B, 2015, 91, .	3.2	58
63	Ambient-Pressure Polymerization of Carbon Anions in the High-Pressure Phase Mg₂C. Inorganic Chemistry, 2015, 54, 10761-10765.	4.0	4
64	Structures and stability of novel transition-metal<mml:math		

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73	Reconstructive structural phase transitions in dense Mg. Journal of Physics Condensed Matter, 2012, 24, 265401.	1.8	10
74	Structural phase transitions in Si under hydrostatic and uniaxial compression. Physical Review B, 2012, 85, .	3.2	12
75	Metallization of solid hydrogen: the challenge and possible solutions. Physical Chemistry Chemical Physics, 2011, 13, 16999.	2.8	23
76	BH3under Pressure: Leaving the Molecular Diborane Motif. Journal of the American Chemical Society, 2011, 133, 21002-21009.	13.7	31
77	Pressure-Induced Formation of Molecular B2X4(Î¼-X)2(X = Cl, Br, I) Species. Inorganic Chemistry, 2011, 50, 10472-10475.	4.0	9
78	Prediction of a bccâ€“hcp phase transition for Sn: A first-principles study. Solid State Communications, 2011, 151, 1873-1873.	1.9	9
79	Silane plus molecular hydrogen as a possible pathway to metallic hydrogen. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 20893-20898.	7.1	38
80	Stability of simple cubic calcium at high pressure: A first-principles study. Physical Review B, 2010, 82, .	3.2	23
81	Consecutive Peierls distortions and high-pressure phase transitions in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>YH</mml:mtext></mml:mrow><mml:mn>3</mml:mn></mml:msu Physical Review B, 2010, 81, .	3.2	23
82	Core effects on the energetics of solid Li at high pressure. Physical Review B, 2009, 79, .	3.2	5
83	Structures of Insulating Phases of Dense Lithium. Physical Review Letters, 2009, 102, 115503.	7.8	70
84	Superconductivity in lithium under high pressure investigated with density functional and Eliashberg theory. Physical Review B, 2009, 79, .	3.2	48
85	Structural Prediction and Phase Transformation Mechanisms in Calcium at High Pressure. Physical Review Letters, 2009, 103, 055503.	7.8	65
86	Structure and electronic properties of at high pressure. Solid State Communications, 2009, 149, 1944-1946.	1.9	26
87	Structure and spectroscopic properties of dense solid hydrogen at 160ÂGPa. Solid State Communications, 2008, 145, 5-10.	1.9	22
88	Electronic structure ofÎ¼-oxygen at high pressure: GW calculations. Physical Review B, 2008, 78, .	3.2	8
89	Pressure-induced structural transformation in solid xenon studied by Raman spectroscopy. Physical Review B, 2008, 77, .	3.2	8
90	Metastable high-pressure single-bonded phases of nitrogen predicted via genetic algorithm. Physical Review B, 2008, 77, .	3.2	65

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91	Superconductivity in high-pressure solids. Journal of Physics Condensed Matter, 2007, 19, 425208.	1.8	11