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	Crystalline LiN₅ Predicted from First-Principles as a Possible High-Energy Material. Journal of Physical Chemistry Letters, 2015, 6, 2363-2366.	4.6	145
2	Pressure-Induced Polymorphic, Optical, and Electronic Transitions of Formamidinium Lead Iodide Perovskite. Journal of Physical Chemistry Letters, 2017, 8, 2119-2125.	4.6	115
3	Design Principles for High-Temperature Superconductors with a Hydrogen-Based Alloy Backbone at Moderate Pressure. Physical Review Letters, 2022, 128, 047001.	7.8	91
4	Nitrogen in black phosphorus structure. Science Advances, 2020, 6, eaba9206.	10.3	90
5	Stable Calcium Nitrides at Ambient and High Pressures. Inorganic Chemistry, 2016, 55, 7550-7555.	4.0	88
6	Hydrogen Pentagraphenelike Structure Stabilized by Hafnium: A High-Temperature Conventional Superconductor. Physical Review Letters, 2020, 125, 217001.	7.8	87
7	A New Allotrope of Nitrogen as High-Energy Density Material. Journal of Physical Chemistry A, 2016, 120, 2920-2925.	2.5	73
8	Structures of Insulating Phases of Dense Lithium. Physical Review Letters, 2009, 102, 115503.	7.8	70
9	Metastable high-pressure single-bonded phases of nitrogen predicted via genetic algorithm. Physical Review B, 2008, 77, .	3.2	65
10	Structural Prediction and Phase Transformation Mechanisms in Calcium at High Pressure. Physical Review Letters, 2009, 103, 055503.	7.8	65
11	Exotic stable cesium polynitrides at high pressure. Scientific Reports, 2015, 5, 16902.	3.3	58
12	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
13	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
14	Metallization and superconductivity of BeH2 under high pressure. Journal of Chemical Physics, 2014, 140, 124707.	3.0	50
15	Superconductivity in lithium under high pressure investigated with density functional and Eliashberg theory. Physical Review B, 2009, 79, .	3.2	48
16	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></mml:math>. Physical Review B, 2017, 96, .	3.2	45
17	Revealing the formation mechanism of ultrahard nanotwinned diamond from onion carbon. Carbon, 2018, 129, 159-167.	10.3	40
18	Synthesis of Xenon and Iron-Nickel Intermetallic Compounds at Earthâ€™s Core Thermodynamic Conditions. Physical Review Letters, 2018, 120, 096001.	7.8	39

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19	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
20	Single-bonded allotrope of nitrogen predicted at high pressure. Physical Review B, 2017, 96, .	3.2	36
21	Superconducting Hydrogen Sulfide. Chemistry - A European Journal, 2018, 24, 1769-1778.	3.3	32
22	BH3under Pressure: Leaving the Molecular Diborane Motif. Journal of the American Chemical Society, 2011, 133, 21002-21009.	13.7	31
23	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
24	B4â”'B1phase transition of GaN under isotropic and uniaxial compression. Physical Review B, 2013, 88, .	3.2	27
25	Structure and electronic properties of at high pressure. Solid State Communications, 2009, 149, 1944-1946.	1.9	26
26	Superconducting Zirconium Polyhydrides at Moderate Pressures. Journal of Physical Chemistry Letters, 2020, 11, 646-651.	4.6	26
27	Dihydrogen Bonding in Compressed Ammonia Borane and Its Roles in Structural Stability. Journal of Physical Chemistry C, 2014, 118, 29591-29598.	3.1	24
28	Stability of simple cubic calcium at high pressure: A first-principles study. Physical Review B, 2010, 82, .	3.2	23
29	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
30	Metallization of solid hydrogen: the challenge and possible solutions. Physical Chemistry Chemical Physics, 2011, 13, 16999.	2.8	23
31	New multifunctional tungsten nitride with energetic N ₆ and extreme hardness predicted from first principles. Europhysics Letters, 2017, 118, 46001.	2.0	23
32	Structure and spectroscopic properties of dense solid hydrogen at 160ÂGPa. Solid State Communications, 2008, 145, 5-10.	1.9	22
33	Modulated Structure Calculated for Superconducting Hydrogen Sulfide. Angewandte Chemie - International Edition, 2017, 56, 11390-11393.	13.8	21
34	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></mm Physical Review B, 2016, 93, .	3.2	20
35	Stable structures of tantalum at high temperature and high pressure. Physical Review B, 2013, 88, .	3.2	19
36	Piezochromism and structural and electronic properties of benz[a]anthracene under pressure. Physical Chemistry Chemical Physics, 2017, 19, 6216-6223.	2.8	19

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37	Hydrogen segregation and its roles in structural stability and metallization: silane under pressure. Scientific Reports, 2015, 5, 13039.	3.3	17
38	Theoretical Predictions of Novel Superconducting Phases of BaGe3 Stable at Atmospheric and High Pressures. Inorganic Chemistry, 2015, 54, 2875-2884.	4.0	17
39	Quantum and Classical Proton Diffusion in Superconducting Clathrate Hydrides. Physical Review Letters, 2021, 126, 117002.	7.8	17
40	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
41	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
42	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
43	Crystal structures of transition metal pernitrides predicted from first principles. RSC Advances, 2018, 8, 36412-36421.	3.6	15
44	Machine learning metadynamics simulation of reconstructive phase transition. Physical Review B, 2021, 103, .	3.2	15
45	Using coherent phonons for ultrafast control of the Dirac node of SrMnSb2. Physical Review B, 2018, 98, .	3.2	14
46	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
47	Structural phase transitions in Si under hydrostatic and uniaxial compression. Physical Review B, 2012, 85, .	3.2	12
48	Mechanism for the Structural Transformation to the Modulated Superconducting Phase of Compressed Hydrogen Sulfide. Scientific Reports, 2019, 9, 5023.	3.3	12
49	o-C240: a new sp3-dominated allotrope of carbon. Journal of Physics Condensed Matter, 2020, 32, 395401.	1.8	12
50	Solid Nitrogen and Nitrogenâ€Rich Compounds as Highâ€Energyâ€Density Materials. Physica Status Solidi (B): Basic Research, 2021, 258, 2000588.	1.5	12
51	Superconductivity in high-pressure solids. Journal of Physics Condensed Matter, 2007, 19, 425208.	1.8	11
52	Thermodynamic ground state of MgB6 predicted from first principles structure search methods. Journal of Chemical Physics, 2014, 140, 044710.	3.0	11
53	IrN4 and IrN7 as potential high-energy-density materials. Journal of Chemical Physics, 2021, 154, 054706.	3.0	11
54	Reconstructive structural phase transitions in dense Mg. Journal of Physics Condensed Matter, 2012, 24, 265401.	1.8	10

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55	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
56	Pressure-Induced Formation of Molecular B2X4(Î¼-X)2(X = Cl, Br, I) Species. Inorganic Chemistry, 2011, 50, 10472-10475.	4.0	9
57	Prediction of a bccâ€“hcp phase transition for Sn: A first-principles study. Solid State Communications, 2011, 151, 1873-1873.	1.9	9
58	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
59	Pressure-induced structural transformations and new polymorphs in BiVO₄. Physical Chemistry Chemical Physics, 2020, 22, 10238-10246.	2.8	9
60	Pressure-induced decomposition of binary lanthanum intermetallic compounds. Physical Review B, 2020, 101, .	3.2	9
61	Electronic structure ofÎ¼-oxygen at high pressure: GW calculations. Physical Review B, 2008, 78, .	3.2	8
62	Pressure-induced structural transformation in solid xenon studied by Raman spectroscopy. Physical Review B, 2008, 77, .	3.2	8
63	Hidden Thermodynamic Ground State of Calcium Diazenide. Journal of Physical Chemistry C, 2014, 118, 650-656. Structures and stability of novel transition-metal<mml:math	3.1	8
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73	Potassium-activated anionic copper and covalent Cuâ€“Cu bonding in compressed Kâ€“Cu compounds. Journal of Chemical Physics, 2021, 154, 134708.	3.0	5
74	Ambient-Pressure Polymerization of Carbon Anions in the High-Pressure Phase Mg₂C. Inorganic Chemistry, 2015, 54, 10761-10765.	4.0	4
75	Modulated Structure Calculated for Superconducting Hydrogen Sulfide. Angewandte Chemie, 2017, 129, 11548-11551.	2.0	4
76	Prediction of a stable helium-hydrogen compound: First-principles simulations. Physical Review B, 2021, 104, .	3.2	4
77	First-principles investigation of rhodium hydrides under high pressure. Physical Review B, 2021, 104, .	3.2	4
78	High-enthalpy crystalline phases of cadmium telluride. Physical Review Research, 2020, 2, .	3.6	4
79	Pressure induced dimer to ionic insulator and metallic structural changes in Al2Br6. Journal of Chemical Physics, 2013, 138, 094501.	3.0	2
80	High pressure structural changes in aluminium triiodide: A first principles study. Journal of Chemical Physics, 2016, 144, 124507.	3.0	2
81	High-pressure phase transition of alkali metalâ€“transition metal deuteride Li2PdD2. Journal of Chemical Physics, 2017, 146, 234506.	3.0	2
82	Stable BaCl solid at high pressure: Prediction and characterization using first principles approach. Journal of Applied Physics, 2017, 122, 235902.	2.5	2
83	Synthesis of superconducting SbS and SbS2 antimony chalcogenide compounds at high pressures. Physical Review B, 2021, 103, .	3.2	2
84	Dirac nodal-line semimetal zinc polynitride at high pressure. Physical Review B, 2022, 105, .	3.2	2
85	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
86	Novel boron channel-based structure of boron carbide at high pressures. Journal of Physics Condensed Matter, 2017, 29, 455401.	1.8	1
87	Oxysulfide Li2BeSO: A potential new material for solid electrolyte predicted from first principles. Journal of Alloys and Compounds, 2020, 818, 152844.	5.5	1
88	High-pressure structural study of Î± -Mn: Experiments and calculations. Physical Review B, 2021, 103, .	3.2	1
89	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
90	Frontispiece: Superconducting Hydrogen Sulfide. Chemistry - A European Journal, 2018, 24, .	3.3	0

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91	Structural diversity and unusual valence states in compressed Na-Hg system. Computational Materials Science, 2022, 211, 111561.	3.0	0