Yanchao Wang

List of Publications by Year
in descending order

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125 papers	11,731 citations	66343 42 h-index	27406 106 g-index
126 all docs	126 docs citations	126 times ranked	6355 citing authors

#	Article	IF	Citations
1	CALYPSO: A method for crystal structure prediction. Computer Physics Communications, 2012, 183, 2063-2070.	7.5	2,085
2	Crystal structure prediction via particle-swarm optimization. Physical Review B, 2010, 82, .	3.2	1,870
3	Predicted Novel High-Pressure Phases of Lithium. Physical Review Letters, 2011, 106, 015503.	7.8	499
4	Particle-swarm structure prediction on clusters. Journal of Chemical Physics, 2012, 137, 084104.	3.0	453
5	Report on the sixth blind test of organic crystal structure prediction methods. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2016, 72, 439-459.	1.1	445
6	Materials discovery at high pressures. Nature Reviews Materials, 2017, 2, .	48.7	427
7	Substitutional Alloy of Bi and Te at High Pressure. Physical Review Letters, 2011, 106, 145501.	7.8	363
8	An effective structure prediction method for layered materials based on 2D particle swarm optimization algorithm. Journal of Chemical Physics, 2012, 137, 224108.	3.0	275
9	Pressure-stabilized superconductive yttrium hydrides. Scientific Reports, 2015, 5, 9948.	3.3	257
10	Predicting Two-Dimensional Boronâ€“Carbon Compounds by the Global Optimization Method. Journal of the American Chemical Society, 2011, 133, 16285-16290.	13.7	242
11	Interface structure prediction via CALYPSO method. Science Bulletin, 2019, 64, 301-309.	9.0	219
12	High pressure partially ionic phase of water ice. Nature Communications, 2011, 2, 563.	12.8	208
13	Superhard<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>BC</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math>in Cubic Diamond Structure. Physical Review Letters, 2015, 114, 015502.	7.8	180
14	Cagelike Diamondoid Nitrogen at High Pressures. Physical Review Letters, 2012, 109, 175502.	7.8	176
15	First-principles structural design of superhard materials. Journal of Chemical Physics, 2013, 138, 114101.	3.0	176
16	Self-assembled ultrathin nanotubes on diamond (100) surface. Nature Communications, 2014, 5, 3666.	12.8	164
17	B₃₈: an all-boron fullerene analogue. Nanoscale, 2014, 6, 11692-11696.	5.6	153
18	Crystal Structures and Exotic Behavior of Magnesium under Pressure. Journal of Physical Chemistry C, 2010, 114, 21745-21749.	3.1	146

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19	CALYPSO structure prediction method and its wide application. Computational Materials Science, 2016, 112, 406-415.	3.0	138
20	Perspective: Crystal structure prediction at high pressures. Journal of Chemical Physics, 2014, 140, 040901.	3.0	135
21	Spiral chain O ₄ form of dense oxygen. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 751-753.	7.1	111
22	Electronic nature of chiral charge order in the kagome superconductor <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Cs</mml:mi><mml:msub><mml:mi mathvariant="normal">V</mml:mi><mml:mn>3</mml:mn></mml:msub><mml:msub><mml:mi>Sb</mml:mi><mml:mn>5</mml:mn></</mml:mi> Physical Review B, 2021, 104, .	3.2	108
23	Enhanced thermoelectric performance of PbTe within the orthorhombic<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>P</mml:mi><mml:mi>n</mml:mi><mml:mi>m</mml:mi><mml:mi>a</mml:mi></mml:mrow></mml:mi> Physical Review B, 2007, 76, .	3.2	107
24	Gold as a 6p-Element in Dense Lithium Aurides. Journal of the American Chemical Society, 2016, 138, 4046-4052.	13.7	101
25	Materials discovery via CALYPSO methodology. Journal of Physics Condensed Matter, 2015, 27, 203203.	1.8	93
26	Electrical Control of Magnetic Phase Transition in a Type-I Multiferroic Double-Metal Trihalide Monolayer. Physical Review Letters, 2020, 124, 067602.	7.8	84
27	High-Temperature Ferromagnetism in an Fe₃P Monolayer with a Large Magnetic Anisotropy. Journal of Physical Chemistry Letters, 2019, 10, 2733-2738.	4.6	79
28	Accelerating CALYPSO structure prediction by data-driven learning of a potential energy surface. Faraday Discussions, 2018, 211, 31-43.	3.2	76
29	Metallic Icosahedron Phase of Sodium at Terapascal Pressures. Physical Review Letters, 2015, 114, 125501.	7.8	75
30	Two-dimensional boronâ€“nitrogenâ€“carbon monolayers with tunable direct band gaps. Nanoscale, 2015, 7, 12023-12029.	5.6	74
31	Stabilization of fullerene-like boron cages by transition metal encapsulation. Nanoscale, 2015, 7, 10482-10489.	5.6	72
32	Phase Diagram and High-Temperature Superconductivity of Compressed Selenium Hydrides. Scientific Reports, 2015, 5, 15433.	3.3	71
33	Computer-Assisted Inverse Design of Inorganic Electrides. Physical Review X, 2017, 7, .	8.9	70
34	Two-dimensional Blue-AsP monolayers with tunable direct band gap and ultrahigh carrier mobility show promising high-performance photovoltaic properties. Nanoscale, 2019, 11, 8260-8269.	5.6	70
35	Orthorhombic C32: a novel superhard sp3 carbon allotrope. Physical Chemistry Chemical Physics, 2013, 15, 14120.	2.8	62
36	A Stable, Magnetic, and Metallic Li3O4Compound as a Discharge Product in a Liâ€“Air Battery. Journal of Physical Chemistry Letters, 2014, 5, 2516-2521.	4.6	52

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37	High-Pressure Phase Transitions and Structures of Topological Insulator BiTeI. Journal of Physical Chemistry C, 2013, 117, 25677-25683.	3.1	50
38	Stable xenon nitride at high pressures. Physical Review B, 2015, 92, .	3.2	50
39	A two-dimensional TiB₄monolayer exhibits planar octacoordinate Ti. Nanoscale, 2017, 9, 17983-17990.	5.6	50
40	N₂H: a novel polymeric hydronitrogen as a high energy density material. Journal of Materials Chemistry A, 2015, 3, 4188-4194.	10.3	49
41	Two-Dimensional C₄N Global Minima: Unique Structural Topologies and Nanoelectronic Properties. Journal of Physical Chemistry C, 2017, 121, 2669-2674.	3.1	49
42	Direct-gap semiconducting tri-layer silicene with 29% photovoltaic efficiency. Nano Energy, 2018, 51, 489-495.	16.0	46
43	Combining Machine Learning Potential and Structure Prediction for Accelerated Materials Design and Discovery. Journal of Physical Chemistry Letters, 2020, 11, 8710-8720.	4.6	45
44	Absence of superconductivity in the high-pressure polymorph of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>MgB</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:ms Physical Review B, 2009, 79, .	3.2	43
45	Pressure-Stabilized Semiconducting Electrides in Alkaline-Earth-Metal Subnitrides. Journal of the American Chemical Society, 2017, 139, 13798-13803.	13.7	43
46	Efficient potential-tuning strategy through p-type doping for designing cathodes with ultrahigh energy density. National Science Review, 2020, 7, 1768-1775.	9.5	43
47	ATLAS: A real-space finite-difference implementation of orbital-free density functional theory. Computer Physics Communications, 2016, 200, 87-95.	7.5	42
48	Unexpected Trend in Stability of Xeâ€“F Compounds under Pressure Driven by Xeâ€“Xe Covalent Bonds. Journal of Physical Chemistry Letters, 2016, 7, 4562-4567.	4.6	41
49	Polyethylene Glycolâ€“Na⁺ Interface of Vanadium Hexacyanoferrate Cathode for Highly Stable Rechargeable Aqueous Sodium-Ion Battery. ACS Applied Materials & Interfaces, 2019, 11, 28762-28768.	8.0	41
50	A symmetry-orientated divide-and-conquer method for crystal structure prediction. Journal of Chemical Physics, 2022, 156, 014105.	3.0	40
51	Structural morphologies of high-pressure polymorphs of strontium hydrides. Physical Chemistry Chemical Physics, 2015, 17, 19379-19385.	2.8	39
52	High Thermoelectric Performance of Ge/Si Coreâ^'Shell Nanowires: First-Principles Prediction. Journal of Physical Chemistry C, 2010, 114, 9096-9100.	3.1	36
53	Structure Prediction of Atoms Adsorbed on Two-Dimensional Layer Materials: Method and Applications. Journal of Physical Chemistry C, 2015, 119, 20111-20118.	3.1	36
54	A hypervalent and cubically coordinated molecular phase of IF₈predicted at high pressure. Chemical Science, 2019, 10, 2543-2550.	7.4	36

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55	Stabilization of ammonia-rich hydrate inside icy planets. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 9003-9008.	7.1	35
56	Stable Lithium Argon compounds under high pressure. Scientific Reports, 2015, 5, 16675.	3.3	34
57	CaCl2-type high-pressure phase of magnesium hydride predicted byab initiophonon calculations. Physical Review B, 2007, 75, .	3.2	33
58	Construction of crystal structure prototype database: methods and applications. Journal of Physics Condensed Matter, 2017, 29, 165901.	1.8	31
59	Computer-Assisted Design of a Superior Be₂BO₃F Deep-Ultraviolet Nonlinear-Optical Material. Inorganic Chemistry, 2018, 57, 5716-5719.	4.0	31
60	X-ray diffraction data-assisted structure searches. Computer Physics Communications, 2017, 213, 40-45.	7.5	30
61	Anatase (101)-like Structural Model Revealed for Metastable Rutile TiO₂(011) Surface. ACS Applied Materials & Interfaces, 2017, 9, 7891-7896.	8.0	29
62	Nonmetallic FeH₆ under High Pressure. Journal of Physical Chemistry C, 2018, 122, 12022-12028.	3.1	29
63	The CALYPSO methodology for structure prediction*. Chinese Physics B, 2019, 28, 106105.	1.4	28
64	High-pressure phase transitions of solid HF, HCl, and HBr: Anab initioevolutionary study. Physical Review B, 2010, 82, .	3.2	27
65	Unexpected and enhanced electrostatic adsorption capacity of oxygen vacancy-rich cobalt-doped In2O3 for high-sensitive MEMS toluene sensor. Sensors and Actuators B: Chemical, 2021, 342, 129949.	7.8	26
66	Origin of the High Thermoelectric Performance in Si Nanowires: A First-Principle Study. Journal of Physical Chemistry C, 2009, 113, 14001-14005.	3.1	25
67	Exotic Hydrogen Bonding in Compressed Ammonia Hydrides. Journal of Physical Chemistry Letters, 2019, 10, 2761-2766.	4.6	25
68	First-principles study of the pressure-induced rutileâ€“CaCl2 phase transition in MgF2. Solid State Communications, 2008, 145, 283-287.	1.9	23
69	Effects of manganese doping on the structure evolution of small-sized boron clusters. Journal of Physics Condensed Matter, 2017, 29, 265401.	1.8	23
70	Large-scale ab initio simulations for periodic system. Computer Physics Communications, 2018, 233, 78-83.	7.5	23
71	Stability of H3O at extreme conditions and implications for the magnetic fields of Uranus and Neptune. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 5638-5643.	7.1	23
72	First-principle optimal local pseudopotentials construction via optimized effective potential method. Journal of Chemical Physics, 2016, 144, 134108.	3.0	22

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73	Novel phases in ammonia-water mixtures under pressure. Journal of Chemical Physics, 2018, 149, 234501.	3.0	22
74	Barium in High Oxidation States in Pressure-Stabilized Barium Fluorides. Journal of Physical Chemistry C, 2018, 122, 12448-12453.	3.1	22
75	Pressure stabilization of long-missing bare C6 hexagonal rings in binary sesquicarbides. Chemical Science, 2014, 5, 3936-3940.	7.4	21
76	The exotically stoichiometric compounds in Alâ€“S system under high pressure. Npj Computational Materials, 2020, 6, .	8.7	21
77	Pressure-stabilized divalent ozonide CaO3 and its impact on Earthâ€™s oxygen cycles. Nature Communications, 2020, 11, 4702.	12.8	20
78	Nonlocal kinetic energy density functionals for isolated systems obtained via local density approximation kernels. Physical Review B, 2020, 101, .	3.2	20
79	Superconductivity of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>MgB</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math> ultrahigh pressure: A first-principles study. Physical Review B, 2009, 80, .	3.2	19
80	Crystal Structures and Electronic Properties of Oxygen-rich Titanium Oxides at High Pressure. Inorganic Chemistry, 2018, 57, 3254-3260.	4.0	19
81	Silicon Framework-Based Lithium Silicides at High Pressures. ACS Applied Materials & Interfaces, 2016, 8, 16761-16767.	8.0	17
82	High pressure structures of â€œ111â€•type iron-based superconductors predicted from first-principles. Physical Chemistry Chemical Physics, 2012, 14, 15029.	2.8	16
83	Ten-fold coordinated polymorph and metallization of TiO₂under high pressure. RSC Advances, 2015, 5, 54253-54257.	3.6	16
84	A hidden symmetry-broken phase of MoS₂ revealed as a superior photovoltaic material. Journal of Materials Chemistry A, 2018, 6, 16087-16093.	10.3	16
85	Local Carbon Concentration Determines the Graphene Edge Structure. Journal of Physical Chemistry Letters, 2020, 11, 3451-3457.	4.6	16
86	Hard and superconducting cubic boron phase via swarm-intelligence structural prediction driven by a machine-learning potential. Physical Review B, 2021, 103, .	3.2	16
87	New Pressure Stabilization Structure in Two-Dimensional PtSe₂. Journal of Physical Chemistry Letters, 2020, 11, 7342-7349.	4.6	15
88	Machine learning metadynamics simulation of reconstructive phase transition. Physical Review B, 2021, 103, .	3.2	15
89	Porous silaphosphorene, silaarsenene and silaantimonene: a sweet marriage of Si and P/As/Sb. Journal of Materials Chemistry A, 2018, 6, 3738-3746.	10.3	14
90	Monoclinic high-pressure polymorph of AlOOH predicted from first principles. Physical Review B, 2016, 94, .	3.2	13

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91	Novel structures of oxygen adsorbed on a Zr(0001) surface predicted from first principles. Applied Surface Science, 2017, 393, 422-427.	6.1	13
92	Nonlocal kinetic energy density functional via line integrals and its application to orbital-free density functional theory. Physical Review B, 2019, 100, .	3.2	13
93	Disproportionation of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>SO</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math> at High Pressure and Temperature. Physical Review Letters, 2022, 128, 106001.	7.8	13
94	An automated predictor for identifying transition states in solids. Npj Computational Materials, 2020, 6, .	8.7	12
95	Particle Swarm Predictions of a SrB₈ Monolayer with 12-Fold Metal Coordination. Journal of the American Chemical Society, 2022, 144, 11120-11128.	13.7	12
96	Prediction of the Xeâ€“He binary phase diagram at high pressures. Chemical Physics Letters, 2015, 640, 115-118.	2.6	11
97	Ab initio electronic structure calculations using a real-space Chebyshev-filtered subspace iteration method. Journal of Physics Condensed Matter, 2019, 31, 455901.	1.8	11
98	Ba with Unusual Oxidation States in Ba Chalcogenides under Pressure. Journal of Physical Chemistry Letters, 2021, 12, 4203-4210.	4.6	11
99	Structure search of two-dimensional systems using CALYPSO methodology. Frontiers of Physics, 2022, 17, 1.	5.0	11
100	Nonlocal pseudopotential energy density functional for orbital-free density functional theory. Nature Communications, 2022, 13, 1385.	12.8	10
101	Pressure-induced amorphization in mayenite (12CaOÂ·7Al2O3). Journal of Chemical Physics, 2011, 135, 094506.	3.0	9
102	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi mathvariant="script">PT</mml:mi></mml:math> -symmetry-protected Dirac states in strain-induced hidden <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Mo</mml:mi><mml:msub><mml:mi mathvariant="normal">S</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math> monolayer. Physical Review B, 2019, 100, .	3.2	9
103	Publisherâ€™s Note: Computer-Assisted Inverse Design of Inorganic Electrides [Phys. Rev. X 7 , 011017 (2017)]. Physical Review X, 2017, 7, .	8.9	8
104	O (N log N) scaling method to evaluate the ionâ€“electron potential of crystalline solids. Journal of Chemical Physics, 2016, 145, 184110.	3.0	7
105	Ground-State Crystal Structure of Strontium Peroxide Predicted from First Principles. Inorganic Chemistry, 2017, 56, 7545-7549.	4.0	7
106	A database assisted protein structure prediction method via a swarm intelligence algorithm. RSC Advances, 2017, 7, 39869-39876.	3.6	7
107	Understanding the Increasing Trend of Sensor Signal with Decreasing Oxygen Partial Pressure by a Sensing-Reaction Model Based on O^{2â€“} Species. ACS Sensors, 2022, 7, 1095-1104.	7.8	7
108	CALYPSO Method for Structure Prediction and Its Applications to Materials Discovery. , 2019, , 1-28.		6

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109	Stabilization of S3O4 at high pressure: implications for the sulfur-excess paradox. Science Bulletin, 2022, 67, 971-976.	9.0	6
110	Pressure-induced structural changes and elemental dissociation of cadmium and mercury chalcogenides. RSC Advances, 2015, 5, 104426-104432.	3.6	5
111	CALYPSO structure prediction method. Chinese Science Bulletin, 2015, 60, 2580-2587.	0.7	5
112	Design of a powered ankle-foot prosthesis with an adjustable stiffness toe joint. Advanced Robotics, 2020, 34, 689-697.	1.8	4
113	High-pressure polymorphs of Li2BeH4predicted by first-principles calculations. Journal of Physics Condensed Matter, 2009, 21, 385405.	1.8	3
114	Pressure-induced reappearance of superconductivity in the oC24 phase of lithium. Solid State Communications, 2016, 225, 7-11.	1.9	3
115	Two-dimensional aluminum monoxide nanosheets: A computational study. Frontiers of Physics, 2018, 13, 1.	5.0	3
116	Prediction of a novel high-pressure phase of hydrogen peroxide. Physical Review B, 2020, 101, .	3.2	3
117	CALYPSO Method for Structure Prediction and Its Applications to Materials Discovery. , 2020, , 2729-2756.		3
118	Ti-fraction-induced electronic and magnetic transformations in titanium oxide films. Journal of Chemical Physics, 2019, 150, 154704.	3.0	2
119	Stability of Ca(OH)2 at Earth's deep lower mantle conditions. Physical Review B, 2021, 104, .	3.2	2
120	Synthesis of calcium polysulfides at high pressures. Physical Review B, 2021, 104, .	3.2	2
121	Stability of the peroxide group in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Ba</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math> under high pressure. Physical Review B, 2021, 103, .	3.2	1
122	A short-range disordered defect in the double layer ice. Journal of Molecular Liquids, 2021, 336, 116356.	4.9	1
123	Zeeman-type energy level splittings controlled by an electric field. Physical Review B, 2022, 106, .	3.2	1
124	Magnetically controllable band splittings in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>P</mml:mi><mml:mi>n</mml:mi><mml:mi>m</mml:mi> ferromagnetic materials. Physical Review B, 2022, 105, .	3.2	0
125	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Ba</mml:mi><mml:msub><mml:mi mathvariant="normal">S</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math> phase featuring v-shape <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">S</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math> unit at high pressure. Physical Review Research, 2022, 4, .	3.6	0