Yanchao Wang

List of Publications by Year
in descending order

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	Structure search of two-dimensional systems using CALYPSO methodology. Frontiers of Physics, 2022, 17, 1.	5.0	11
2	A symmetry-orientated divide-and-conquer method for crystal structure prediction. Journal of Chemical Physics, 2022, 156, 014105.	3.0	40
3	Stabilization of S3O4 at high pressure: implications for the sulfur-excess paradox. Science Bulletin, 2022, 67, 971-976.	9.0	6
4	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
5	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> at High Pressure and Temperature. Physical Review Letters, 2022, 128, 106001.	7.8	13
6	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
7	Nonlocal pseudopotential energy density functional for orbital-free density functional theory. Nature Communications, 2022, 13, 1385.	12.8	10
8	Semiconducting <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
9	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
10	Zeeman-type energy level splittings controlled by an electric field. Physical Review B, 2022, 106, .	3.2	1
11	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
12	Machine learning metadynamics simulation of reconstructive phase transition. Physical Review B, 2021, 103, .	3.2	15
13	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
14	Ba with Unusual Oxidation States in Ba Chalcogenides under Pressure. Journal of Physical Chemistry Letters, 2021, 12, 4203-4210.	4.6	11
15	Stability of Ca(OH)2 at Earth's deep lower mantle conditions. Physical Review B, 2021, 104, .	3.2	2
16	A short-range disordered defect in the double layer ice. Journal of Molecular Liquids, 2021, 336, 116356.	4.9	1
17	Synthesis of calcium polysulfides at high pressures. Physical Review B, 2021, 104, .	3.2	2
18	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></ Physical Review B, 2021, 104, .	3.2	108

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19	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
20	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
21	New Pressure Stabilization Structure in Two-Dimensional PtSe₂. Journal of Physical Chemistry Letters, 2020, 11, 7342-7349.	4.6	15
22	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
23	Pressure-stabilized divalent ozonide CaO3 and its impact on Earthâ€™s oxygen cycles. Nature Communications, 2020, 11, 4702.	12.8	20
24	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
25	Nonlocal kinetic energy density functionals for isolated systems obtained via local density approximation kernels. Physical Review B, 2020, 101, .	3.2	20
26	An automated predictor for identifying transition states in solids. Npj Computational Materials, 2020, 6, .	8.7	12
27	The exotically stoichiometric compounds in Alâ€“S system under high pressure. Npj Computational Materials, 2020, 6, .	8.7	21
28	Electrical Control of Magnetic Phase Transition in a Type-I Multiferroic Double-Metal Trihalide Monolayer. Physical Review Letters, 2020, 124, 067602.	7.8	84
29	Prediction of a novel high-pressure phase of hydrogen peroxide. Physical Review B, 2020, 101, .	3.2	3
30	Design of a powered ankle-foot prosthesis with an adjustable stiffness toe joint. Advanced Robotics, 2020, 34, 689-697.	1.8	4
31	Local Carbon Concentration Determines the Graphene Edge Structure. Journal of Physical Chemistry Letters, 2020, 11, 3451-3457.	4.6	16
32	CALYPSO Method for Structure Prediction and Its Applications to Materials Discovery. , 2020, , 2729-2756.		3
33	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
34	The CALYPSO methodology for structure prediction*. Chinese Physics B, 2019, 28, 106105.	1.4	28
35	A hypervalent and cubically coordinated molecular phase of IF₈predicted at high pressure. Chemical Science, 2019, 10, 2543-2550.	7.4	36
36	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

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37	High-Temperature Ferromagnetism in an Fe₃P Monolayer with a Large Magnetic Anisotropy. Journal of Physical Chemistry Letters, 2019, 10, 2733-2738.	4.6	79
38	Exotic Hydrogen Bonding in Compressed Ammonia Hydrides. Journal of Physical Chemistry Letters, 2019, 10, 2761-2766.	4.6	25
39	Ti-fraction-induced electronic and magnetic transformations in titanium oxide films. Journal of Chemical Physics, 2019, 150, 154704.	3.0	2
40	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
41	Interface structure prediction via CALYPSO method. Science Bulletin, 2019, 64, 301-309.	9.0	219
42	<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
43	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
44	CALYPSO Method for Structure Prediction and Its Applications to Materials Discovery. , 2019, , 1-28.		6
45	Crystal Structures and Electronic Properties of Oxygen-rich Titanium Oxides at High Pressure. Inorganic Chemistry, 2018, 57, 3254-3260.	4.0	19
46	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
47	Computer-Assisted Design of a Superior Be₂BO₃F Deep-Ultraviolet Nonlinear-Optical Material. Inorganic Chemistry, 2018, 57, 5716-5719.	4.0	31
48	Accelerating CALYPSO structure prediction by data-driven learning of a potential energy surface. Faraday Discussions, 2018, 211, 31-43.	3.2	76
49	Novel phases in ammonia-water mixtures under pressure. Journal of Chemical Physics, 2018, 149, 234501.	3.0	22
50	Barium in High Oxidation States in Pressure-Stabilized Barium Fluorides. Journal of Physical Chemistry C, 2018, 122, 12448-12453.	3.1	22
51	Direct-gap semiconducting tri-layer silicene with 29% photovoltaic efficiency. Nano Energy, 2018, 51, 489-495.	16.0	46
52	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
53	Large-scale ab initio simulations for periodic system. Computer Physics Communications, 2018, 233, 78-83.	7.5	23
54	Two-dimensional aluminum monoxide nanosheets: A computational study. Frontiers of Physics, 2018, 13, 1.	5.0	3

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55	Nonmetallic FeH₆ under High Pressure. Journal of Physical Chemistry C, 2018, 122, 12022-12028.	3.1	29
56	Two-Dimensional C₄N Global Minima: Unique Structural Topologies and Nanoelectronic Properties. Journal of Physical Chemistry C, 2017, 121, 2669-2674.	3.1	49
57	Materials discovery at high pressures. Nature Reviews Materials, 2017, 2, .	48.7	427
58	Anatase (101)-like Structural Model Revealed for Metastable Rutile TiO₂(011) Surface. ACS Applied Materials & Interfaces, 2017, 9, 7891-7896.	8.0	29
59	Computer-Assisted Inverse Design of Inorganic Electrides. Physical Review X, 2017, 7, .	8.9	70
60	Effects of manganese doping on the structure evolution of small-sized boron clusters. Journal of Physics Condensed Matter, 2017, 29, 265401.	1.8	23
61	Ground-State Crystal Structure of Strontium Peroxide Predicted from First Principles. Inorganic Chemistry, 2017, 56, 7545-7549.	4.0	7
62	Construction of crystal structure prototype database: methods and applications. Journal of Physics Condensed Matter, 2017, 29, 165901.	1.8	31
63	X-ray diffraction data-assisted structure searches. Computer Physics Communications, 2017, 213, 40-45.	7.5	30
64	A two-dimensional TiB₄monolayer exhibits planar octacoordinate Ti. Nanoscale, 2017, 9, 17983-17990.	5.6	50
65	A database assisted protein structure prediction method via a swarm intelligence algorithm. RSC Advances, 2017, 7, 39869-39876.	3.6	7
66	Pressure-Stabilized Semiconducting Electrides in Alkaline-Earth-Metal Subnitrides. Journal of the American Chemical Society, 2017, 139, 13798-13803.	13.7	43
67	Publisherâ€™s Note: Computer-Assisted Inverse Design of Inorganic Electrides [Phys. Rev. X 7 , 011017 (2017)]. Physical Review X, 2017, 7, .	8.9	8
68	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
69	Novel structures of oxygen adsorbed on a Zr(0001) surface predicted from first principles. Applied Surface Science, 2017, 393, 422-427.	6.1	13
70	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
71	Monoclinic high-pressure polymorph of AlOOH predicted from first principles. Physical Review B, 2016, 94, .	3.2	13
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	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
74	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
75	Silicon Framework-Based Lithium Silicides at High Pressures. ACS Applied Materials & Interfaces, 2016, 8, 16761-16767.	8.0	17
76	Pressure-induced reappearance of superconductivity in the oC24 phase of lithium. Solid State Communications, 2016, 225, 7-11.	1.9	3
77	ATLAS: A real-space finite-difference implementation of orbital-free density functional theory. Computer Physics Communications, 2016, 200, 87-95.	7.5	42
78	Gold as a 6p-Element in Dense Lithium Aurides. Journal of the American Chemical Society, 2016, 138, 4046-4052.	13.7	101
79	CALYPSO structure prediction method and its wide application. Computational Materials Science, 2016, 112, 406-415.	3.0	138
80	Prediction of the Xeâ€“He binary phase diagram at high pressures. Chemical Physics Letters, 2015, 640, 115-118.	2.6	11
81	Phase Diagram and High-Temperature Superconductivity of Compressed Selenium Hydrides. Scientific Reports, 2015, 5, 15433.	3.3	71
82	Stable xenon nitride at high pressures. Physical Review B, 2015, 92, .	3.2	50
83	Stable Lithium Argon compounds under high pressure. Scientific Reports, 2015, 5, 16675.	3.3	34
84	Pressure-stabilized superconductive yttrium hydrides. Scientific Reports, 2015, 5, 9948.	3.3	257
85	N₂H: a novel polymeric hydronitrogen as a high energy density material. Journal of Materials Chemistry A, 2015, 3, 4188-4194.	10.3	49
86	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
87	Two-dimensional boronâ€“nitrogenâ€“carbon monolayers with tunable direct band gaps. Nanoscale, 2015, 7, 12023-12029.	5.6	74
88	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
89	Ten-fold coordinated polymorph and metallization of TiO₂under high pressure. RSC Advances, 2015, 5, 54253-54257.	3.6	16
90	Structural morphologies of high-pressure polymorphs of strontium hydrides. Physical Chemistry Chemical Physics, 2015, 17, 19379-19385.	2.8	39

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91	Materials discovery via CALYPSO methodology. Journal of Physics Condensed Matter, 2015, 27, 203203.	1.8	93
92	Metallic Icosahedron Phase of Sodium at Terapascal Pressures. Physical Review Letters, 2015, 114, 125501.	7.8	75
93	Stabilization of fullerene-like boron cages by transition metal encapsulation. Nanoscale, 2015, 7, 10482-10489.	5.6	72
94	Pressure-induced structural changes and elemental dissociation of cadmium and mercury chalcogenides. RSC Advances, 2015, 5, 104426-104432.	3.6	5
95	CALYPSO structure prediction method. Chinese Science Bulletin, 2015, 60, 2580-2587.	0.7	5
96	Perspective: Crystal structure prediction at high pressures. Journal of Chemical Physics, 2014, 140, 040901.	3.0	135
97	Self-assembled ultrathin nanotubes on diamond (100) surface. Nature Communications, 2014, 5, 3666.	12.8	164
98	B₃₈: an all-boron fullerene analogue. Nanoscale, 2014, 6, 11692-11696.	5.6	153
99	Pressure stabilization of long-missing bare C6 hexagonal rings in binary sesquicarbides. Chemical Science, 2014, 5, 3936-3940.	7.4	21
100	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
101	Orthorhombic C32: a novel superhard sp3 carbon allotrope. Physical Chemistry Chemical Physics, 2013, 15, 14120.	2.8	62
102	High-Pressure Phase Transitions and Structures of Topological Insulator BiTeI. Journal of Physical Chemistry C, 2013, 117, 25677-25683.	3.1	50
103	First-principles structural design of superhard materials. Journal of Chemical Physics, 2013, 138, 114101.	3.0	176
104	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
105	High pressure structures of â€œ111â€•type iron-based superconductors predicted from first-principles. Physical Chemistry Chemical Physics, 2012, 14, 15029.	2.8	16
106	Cagelike Diamondoid Nitrogen at High Pressures. Physical Review Letters, 2012, 109, 175502.	7.8	176
107	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
108	Particle-swarm structure prediction on clusters. Journal of Chemical Physics, 2012, 137, 084104.	3.0	453

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109	CALYPSO: A method for crystal structure prediction. Computer Physics Communications, 2012, 183, 2063-2070.	7.5	2,085
110	Predicting Two-Dimensional Boronâ€“Carbon Compounds by the Global Optimization Method. Journal of the American Chemical Society, 2011, 133, 16285-16290.	13.7	242
111	Substitutional Alloy of Bi and Te at High Pressure. Physical Review Letters, 2011, 106, 145501.	7.8	363
112	High pressure partially ionic phase of water ice. Nature Communications, 2011, 2, 563.	12.8	208
113	Predicted Novel High-Pressure Phases of Lithium. Physical Review Letters, 2011, 106, 015503.	7.8	499
114	Pressure-induced amorphization in mayenite (12CaOÂ·7Al2O3). Journal of Chemical Physics, 2011, 135, 094506.	3.0	9
115	Crystal structure prediction via particle-swarm optimization. Physical Review B, 2010, 82, .	3.2	1,870
116	High Thermoelectric Performance of Ge/Si Coreâ^'Shell Nanowires: First-Principles Prediction. Journal of Physical Chemistry C, 2010, 114, 9096-9100.	3.1	36
117	Crystal Structures and Exotic Behavior of Magnesium under Pressure. Journal of Physical Chemistry C, 2010, 114, 21745-21749.	3.1	146
118	High-pressure phase transitions of solid HF, HCl, and HBr: Anab initioevolutionary study. Physical Review B, 2010, 82, .	3.2	27
119	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>under ultrahigh pressure: A first-principles study. Physical Review B, 2009, 80, .	3.2	19
120	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:msub></mml:mrow></mml:math>. Physical Review B, 2009, 79, .	3.2	43
121	High-pressure polymorphs of Li2BeH4predicted by first-principles calculations. Journal of Physics Condensed Matter, 2009, 21, 385405.	1.8	3
122	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
123	First-principles study of the pressure-induced rutileâ€“CaCl2 phase transition in MgF2. Solid State Communications, 2008, 145, 283-287.	1.9	23
124	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:math>. Physical Review B, 2007, 76, .	3.2	107
125	CaCl2-type high-pressure phase of magnesium hydride predicted byab initiophonon calculations. Physical Review B, 2007, 75, .	3.2	33