Yanchao Wang

List of Publications by Year in Descending Order

116 papers	8,658 citations	38 h-index	92 g-index
126 ext. papers	10,333 ext. citations	6.6 avg, IF	6.33 L-index

#	Paper	IF	Citations
116	A symmetry-orientated divide-and-conquer method for crystal structure prediction.. *Journal of Chemical Physics*, **2022**, 156, 014105	3.9	8
115	Structure search of two-dimensional systems using CALYPSO methodology. *Frontiers of Physics*, **2022**, 17, 1	3.7	1
114	Disproportionation of SO_{2} at High Pressure and Temperature.. *Physical Review Letters*, **2022**, 128, 106001	7.4	0
113	Nonlocal pseudopotential energy density functional for orbital-free density functional theory.. *Nature Communications*, **2022**, 13, 1385	17.4	1
112	Ba with Unusual Oxidation States in Ba Chalcogenides under Pressure. *Journal of Physical Chemistry Letters*, **2021**, 12, 4203-4210	6.4	4
111	Hard and superconducting cubic boron phase via swarm-intelligence structural prediction driven by a machine-learning potential. *Physical Review B*, **2021**, 103,	3.3	7
110	Machine learning metadynamics simulation of reconstructive phase transition. *Physical Review B*, **2021**, 103,	3.3	6
109	A short-range disordered defect in the double layer ice. *Journal of Molecular Liquids*, **2021**, 336, 116356	6	
108	Electronic nature of chiral charge order in the kagome superconductor CsV3Sb5. *Physical Review B*, **2021**, 104,	3.3	17
107	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	8.5	10
106	Stability of HO 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	11.5	8
105	Nonlocal kinetic energy density functionals for isolated systems obtained via local density approximation kernels. *Physical Review B*, **2020**, 101,	3.3	13
104	An automated predictor for identifying transition states in solids. *Npj Computational Materials*, **2020**, 6,	10.9	5
103	The exotically stoichiometric compounds in Al□ system under high pressure. *Npj Computational Materials*, **2020**, 6,	10.9	10
102	Electrical Control of Magnetic Phase Transition in a Type-I Multiferroic Double-Metal Trihalide Monolayer. *Physical Review Letters*, **2020**, 124, 067602	7.4	38
101	Prediction of a novel high-pressure phase of hydrogen peroxide. *Physical Review B*, **2020**, 101,	3.3	2
100	Design of a powered ankle-foot prosthesis with an adjustable stiffness toe joint. *Advanced Robotics*, **2020**, 34, 689-697	1.7	2

99	CALYPSO Method for Structure Prediction and Its Applications to Materials Discovery **2020**, 2729-2756		1
98	Efficient potential-tuning strategy through p-type doping for designing cathodes with ultrahigh energy density. *National Science Review*, **2020**, 7, 1768-1775	10.8	23
97	New Pressure Stabilization Structure in Two-Dimensional PtSe. *Journal of Physical Chemistry Letters* , **2020**, 11, 7342-7349	6.4	5
96	Combining Machine Learning Potential and Structure Prediction for Accelerated Materials Design and Discovery. *Journal of Physical Chemistry Letters*, **2020**, 11, 8710-8720	6.4	18
95	Pressure-stabilized divalent ozonide CaO and its impact on Earth's oxygen cycles. *Nature Communications*, **2020**, 11, 4702	17.4	3
94	Local Carbon Concentration Determines the Graphene Edge Structure. *Journal of Physical Chemistry Letters*, **2020**, 11, 3451-3457	6.4	10
93	A hypervalent and cubically coordinated molecular phase of IF predicted at high pressure. *Chemical Science*, **2019**, 10, 2543-2550	9.4	20
92	Ab initio electronic structure calculations using a real-space Chebyshev-filtered subspace iteration method. *Journal of Physics Condensed Matter*, **2019**, 31, 455901	1.8	5
91	High-Temperature Ferromagnetism in an FeP Monolayer with a Large Magnetic Anisotropy. *Journal of Physical Chemistry Letters*, **2019**, 10, 2733-2738	6.4	50
90	Exotic Hydrogen Bonding in Compressed Ammonia Hydrides. *Journal of Physical Chemistry Letters*, **2019**, 10, 2761-2766	6.4	17
89	Ti-fraction-induced electronic and magnetic transformations in titanium oxide films. *Journal of Chemical Physics*, **2019**, 150, 154704	3.9	2
88	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	7.7	38
87	Polyethylene Glycol-Na Interface of Vanadium Hexacyanoferrate Cathode for Highly Stable Rechargeable Aqueous Sodium-Ion Battery. *ACS Applied Materials & Interfaces*, **2019**, 11, 28762-28768	9.5	20
86	The CALYPSO methodology for structure prediction. *Chinese Physics B*, **2019**, 28, 106105	1.2	10
85	Interface structure prediction via CALYPSO method. *Science Bulletin*, **2019**, 64, 301-309	10.6	125
84	PT-symmetry-protected Dirac states in strain-induced hidden MoS2 monolayer. *Physical Review B*, **2019**, 100,	3.3	6
83	Nonlocal kinetic energy density functional via line integrals and its application to orbital-free density functional theory. *Physical Review B*, **2019**, 100,	3.3	6
82	CALYPSO Method for Structure Prediction and Its Applications to Materials Discovery **2019**, 1-28		5

81	Crystal Structures and Electronic Properties of Oxygen-rich Titanium Oxides at High Pressure. *Inorganic Chemistry*, **2018**, 57, 3254-3260	5.1	15
80	Porous silaphosphorene, silaarsenene and silaantimonene: a sweet marriage of Si and P/As/Sb. *Journal of Materials Chemistry A*, **2018**, 6, 3738-3746	13	9
79	Computer-Assisted Design of a Superior BeBOF Deep-Ultraviolet Nonlinear-Optical Material. *Inorganic Chemistry*, **2018**, 57, 5716-5719	5.1	24
78	Accelerating CALYPSO structure prediction by data-driven learning of a potential energy surface. *Faraday Discussions*, **2018**, 211, 31-43	3.6	40
77	A hidden symmetry-broken phase of MoS2 revealed as a superior photovoltaic material. *Journal of Materials Chemistry A*, **2018**, 6, 16087-16093	13	11
76	Large-scale ab initio simulations for periodic system. *Computer Physics Communications*, **2018**, 233, 78-83	4.2	16
75	Two-dimensional aluminum monoxide nanosheets: A computational study. *Frontiers of Physics*, **2018**, 13, 1	3.7	3
74	Nonmetallic FeH6 under High Pressure. *Journal of Physical Chemistry C*, **2018**, 122, 12022-12028	3.8	21
73	Novel phases in ammonia-water mixtures under pressure. *Journal of Chemical Physics*, **2018**, 149, 234501	3.9	18
72	Barium in High Oxidation States in Pressure-Stabilized Barium Fluorides. *Journal of Physical Chemistry C*, **2018**, 122, 12448-12453	3.8	15
71	Direct-gap semiconducting tri-layer silicene with 29% photovoltaic efficiency. *Nano Energy*, **2018**, 51, 489-495	17.1	34
70	Two-Dimensional C4N Global Minima: Unique Structural Topologies and Nanoelectronic Properties. *Journal of Physical Chemistry C*, **2017**, 121, 2669-2674	3.8	37
69	Materials discovery at high pressures. *Nature Reviews Materials*, **2017**, 2,	73.3	266
68	Anatase (101)-like Structural Model Revealed for Metastable Rutile TiO(011) Surface. *ACS Applied Materials & Interfaces*, **2017**, 9, 7891-7896	9.5	22
67	Computer-Assisted Inverse Design of Inorganic Electrides. *Physical Review X*, **2017**, 7,	9.1	51
66	Effects of manganese doping on the structure evolution of small-sized boron clusters. *Journal of Physics Condensed Matter*, **2017**, 29, 265401	1.8	14
65	Ground-State Crystal Structure of Strontium Peroxide Predicted from First Principles. *Inorganic Chemistry*, **2017**, 56, 7545-7549	5.1	3
64	Construction of crystal structure prototype database: methods and applications. *Journal of Physics Condensed Matter*, **2017**, 29, 165901	1.8	17

63	X-ray diffraction data-assisted structure searches. *Computer Physics Communications*, **2017**, 213, 40-45	4.2	21
62	A two-dimensional TiB monolayer exhibits planar octacoordinate Ti. *Nanoscale*, **2017**, 9, 17983-17990	7.7	28
61	A database assisted protein structure prediction method via a swarm intelligence algorithm. *RSC Advances*, **2017**, 7, 39869-39876	3.7	2
60	Pressure-Stabilized Semiconducting Electrides in Alkaline-Earth-Metal Subnitrides. *Journal of the American Chemical Society*, **2017**, 139, 13798-13803	16.4	23
59	Publisher's Note: Computer-Assisted Inverse Design of Inorganic Electrides [Phys. Rev. X 7, 011017 (2017)]. *Physical Review X*, **2017**, 7,	9.1	8
58	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	11.5	26
57	Novel structures of oxygen adsorbed on a Zr(0001) surface predicted from first principles. *Applied Surface Science*, **2017**, 393, 422-427	6.7	10
56	Report on the sixth blind test of organic crystal structure prediction methods. *Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials*, **2016**, 72, 439-59	1.8	338
55	Unexpected Trend in Stability of Xe-F Compounds under Pressure Driven by Xe-Xe Covalent Bonds. *Journal of Physical Chemistry Letters*, **2016**, 7, 4562-4567	6.4	33
54	Silicon Framework-Based Lithium Silicides at High Pressures. *ACS Applied Materials & Interfaces* , **2016**, 8, 16761-7	9.5	11
53	Pressure-induced reappearance of superconductivity in the oC24 phase of lithium. *Solid State Communications*, **2016**, 225, 7-11	1.6	2
52	ATLAS: A real-space finite-difference implementation of orbital-free density functional theory. *Computer Physics Communications*, **2016**, 200, 87-95	4.2	29
51	Gold as a 6p-Element in Dense Lithium Aurides. *Journal of the American Chemical Society*, **2016**, 138, 4046-52	14	70
50	CALYPSO structure prediction method and its wide application. *Computational Materials Science*, **2016**, 112, 406-415	3.2	102
49	O(NlogN) scaling method to evaluate the ion-electron potential of crystalline solids. *Journal of Chemical Physics*, **2016**, 145, 184110	3.9	6
48	Monoclinic high-pressure polymorph of AlOOH predicted from first principles. *Physical Review B*, **2016**, 94,	3.3	9
47	First-principle optimal local pseudopotentials construction via optimized effective potential method. *Journal of Chemical Physics*, **2016**, 144, 134108	3.9	15
46	Two-dimensional boron-nitrogen-carbon monolayers with tunable direct band gaps. *Nanoscale*, **2015**, 7, 12023-9	7.7	63

45	Structure Prediction of Atoms Adsorbed on Two-Dimensional Layer Materials: Method and Applications. *Journal of Physical Chemistry C*, **2015**, 119, 20111-20118	3.8	28
44	Ten-fold coordinated polymorph and metallization of TiO2 under high pressure. *RSC Advances*, **2015**, 5, 54253-54257	3.7	11
43	Structural morphologies of high-pressure polymorphs of strontium hydrides. *Physical Chemistry Chemical Physics*, **2015**, 17, 19379-85	3.6	29
42	Materials discovery via CALYPSO methodology. *Journal of Physics Condensed Matter*, **2015**, 27, 203203	1.8	63
41	Metallic icosahedron phase of sodium at terapascal pressures. *Physical Review Letters*, **2015**, 114, 125501	7.4	56
40	Stabilization of fullerene-like boron cages by transition metal encapsulation. *Nanoscale*, **2015**, 7, 10482-9	7.7	59
39	Pressure-induced structural changes and elemental dissociation of cadmium and mercury chalcogenides. *RSC Advances*, **2015**, 5, 104426-104432	3.7	4
38	Prediction of the Xe□e binary phase diagram at high pressures. *Chemical Physics Letters*, **2015**, 640, 115-118	2.5	7
37	Phase Diagram and High-Temperature Superconductivity of Compressed Selenium Hydrides. *Scientific Reports*, **2015**, 5, 15433	4.9	56
36	Stable xenon nitride at high pressures. *Physical Review B*, **2015**, 92,	3.3	39
35	Stable Lithium Argon compounds under high pressure. *Scientific Reports*, **2015**, 5, 16675	4.9	26
34	Pressure-stabilized superconductive yttrium hydrides. *Scientific Reports*, **2015**, 5, 9948	4.9	184
33	N2H: a novel polymeric hydronitrogen as a high energy density material. *Journal of Materials Chemistry A*, **2015**, 3, 4188-4194	13	42
32	Superhard BC(3) in cubic diamond structure. *Physical Review Letters*, **2015**, 114, 015502	7.4	147
31	CALYPSO structure prediction method. *Chinese Science Bulletin*, **2015**, 60, 2580-2587	2.9	3
30	Perspective: crystal structure prediction at high pressures. *Journal of Chemical Physics*, **2014**, 140, 040901	3.9	116
29	Self-assembled ultrathin nanotubes on diamond (100) surface. *Nature Communications*, **2014**, 5, 3666	17.4	133
28	B38: an all-boron fullerene analogue. *Nanoscale*, **2014**, 6, 11692-6	7.7	127

27	Pressure stabilization of long-missing bare C6 hexagonal rings in binary sesquicarbides. *Chemical Science*, **2014**, 5, 3936-3940	9.4	19
26	A Stable, Magnetic, and Metallic Li3O4 Compound as a Discharge Product in a Li-Air Battery. *Journal of Physical Chemistry Letters*, **2014**, 5, 2516-21	6.4	48
25	Orthorhombic C32: a novel superhard sp3 carbon allotrope. *Physical Chemistry Chemical Physics*, **2013**, 15, 14120-5	3.6	52
24	High-Pressure Phase Transitions and Structures of Topological Insulator BiTeI. *Journal of Physical Chemistry C*, **2013**, 117, 25677-25683	3.8	43
23	First-principles structural design of superhard materials. *Journal of Chemical Physics*, **2013**, 138, 114101	3.9	151
22	An effective structure prediction method for layered materials based on 2D particle swarm optimization algorithm. *Journal of Chemical Physics*, **2012**, 137, 224108	3.9	223
21	High pressure structures of "111" type iron-based superconductors predicted from first-principles. *Physical Chemistry Chemical Physics*, **2012**, 14, 15029-35	3.6	15
20	Cagelike diamondoid nitrogen at high pressures. *Physical Review Letters*, **2012**, 109, 175502	7.4	139
19	Spiral chain O form of dense oxygen. *Proceedings of the National Academy of Sciences of the United States of America*, **2012**, 109, 751-3	11.5	104
18	Particle-swarm structure prediction on clusters. *Journal of Chemical Physics*, **2012**, 137, 084104	3.9	340
17	CALYPSO: A method for crystal structure prediction. *Computer Physics Communications*, **2012**, 183, 2063-2070	4.1	1464
16	Predicting two-dimensional boron-carbon compounds by the global optimization method. *Journal of the American Chemical Society*, **2011**, 133, 16285-90	16.4	209
15	Substitutional alloy of Bi and Te at high pressure. *Physical Review Letters*, **2011**, 106, 145501	7.4	318
14	High pressure partially ionic phase of water ice. *Nature Communications*, **2011**, 2, 563	17.4	201
13	Predicted novel high-pressure phases of lithium. *Physical Review Letters*, **2011**, 106, 015503	7.4	429
12	Pressure-induced amorphization in mayenite (12CaO 7Al2O3). *Journal of Chemical Physics*, **2011**, 135, 094506	3.9	9
11	High Thermoelectric Performance of Ge/Si Core Shell Nanowires: First-Principles Prediction. *Journal of Physical Chemistry C*, **2010**, 114, 9096-9100	3.8	34
10	Crystal Structures and Exotic Behavior of Magnesium under Pressure. *Journal of Physical Chemistry C*, **2010**, 114, 21745-21749	3.8	121

9	High-pressure phase transitions of solid HF, HCl, and HBr: An ab initio evolutionary study. *Physical Review B*, **2010**, 82,	3.3	26
8	Crystal structure prediction via particle-swarm optimization. *Physical Review B*, **2010**, 82,	3.3	1446
7	Superconductivity of MgB2 under ultrahigh pressure: A first-principles study. *Physical Review B*, **2009**, 80,	3.3	12
6	Absence of superconductivity in the high-pressure polymorph of MgB2. *Physical Review B*, **2009**, 79,	3.3	39
5	High-pressure polymorphs of Li(2)BeH(4) predicted by first-principles calculations. *Journal of Physics Condensed Matter*, **2009**, 21, 385405	1.8	3
4	Origin of the High Thermoelectric Performance in Si Nanowires: A First-Principle Study. *Journal of Physical Chemistry C*, **2009**, 113, 14001-14005	3.8	23
3	First-principles study of the pressure-induced rutile□CaCl2 phase transition in MgF2. *Solid State Communications*, **2008**, 145, 283-287	1.6	20
2	CaCl2-type high-pressure phase of magnesium hydride predicted by ab initio phonon calculations. *Physical Review B*, **2007**, 75,	3.3	33
1	Enhanced thermoelectric performance of PbTe within the orthorhombic Pnma phase. *Physical Review B*, **2007**, 76,	3.3	99