Jian Lv

List of Publications by Year in descending order

106 papers	9,840 citations	117625 34 h-index	36028 97 g-index
107 all docs	107 docs citations	107 times ranked	5540 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	Route to a Superconducting Phase above Room Temperature in Electron-Doped Hydride Compounds under High Pressure. Physical Review Letters, 2019, 123, 097001.	7.8	255
10	Interface structure prediction via CALYPSO method. Science Bulletin, 2019, 64, 301-309.	9.0	219
11	High pressure partially ionic phase of water ice. Nature Communications, 2011, 2, 563.	12.8	208
12	Cagelike Diamondoid Nitrogen at High Pressures. Physical Review Letters, 2012, 109, 175502.	7.8	176
13	First-principles structural design of superhard materials. Journal of Chemical Physics, 2013, 138, 114101.	3.0	176
14	B₃₈: an all-boron fullerene analogue. Nanoscale, 2014, 6, 11692-11696.	5.6	153
15	CALYPSO structure prediction method and its wide application. Computational Materials Science, 2016, 112, 406-415.	3.0	138
16	Functionality-Directed Screening of Pb-Free Hybrid Organicâ€“Inorganic Perovskites with Desired Intrinsic Photovoltaic Functionalities. Chemistry of Materials, 2017, 29, 524-538.	6.7	135
17	Perovskite Solar Absorbers: Materials by Design. Small Methods, 2018, 2, 1700316.	8.6	95
18	Materials discovery via CALYPSO methodology. Journal of Physics Condensed Matter, 2015, 27, 203203.	1.8	93

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19	Accelerating CALYPSO structure prediction by data-driven learning of a potential energy surface. Faraday Discussions, 2018, 211, 31-43.	3.2	76
20	Systematic theoretical investigation of geometries, stabilities and magnetic properties of iron oxide clusters (FeO)_n^{Î¼}(n = 1â€“8, Î¼ = 0, Â±1): insights and perspectives. RSC Advances, 2015, 5, 6560-6570.	3.6	74
21	Stabilization of fullerene-like boron cages by transition metal encapsulation. Nanoscale, 2015, 7, 10482-10489.	5.6	72
22	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
23	Geometries, stabilities and fragmental channels of neutral and charged sulfur clusters: S_n^Q(n = 3â€“20, Q = 0, Â±1). Physical Chemistry Chemical Physics, 2015, 17, 13590-13597.	2.8	69
24	Rare Helium-Bearing Compound <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mrow><mml:msub><mml:mrow><mml:mi>FeO</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:mrow></mml:math> Stabilized at Deep-Earth Conditions. Physical Review Letters, 2018, 121, 255703.	7.8	68
25	Ab Initio Search for Global Minimum Structures of Pure and Boron Doped Silver Clusters. Journal of Physical Chemistry A, 2015, 119, 6738-6745.	2.5	62
26	Understanding the structural transformation, stability of medium-sized neutral and charged silicon clusters. Scientific Reports, 2015, 5, 15951.	3.3	52
27	A two-dimensional TiB₄monolayer exhibits planar octacoordinate Ti. Nanoscale, 2017, 9, 17983-17990.	5.6	50
28	Direct-gap semiconducting tri-layer silicene with 29% photovoltaic efficiency. Nano Energy, 2018, 51, 489-495.	16.0	46
29	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
30	A symmetry-orientated divide-and-conquer method for crystal structure prediction. Journal of Chemical Physics, 2022, 156, 014105.	3.0	40
31	Theory-orientated discovery of high-temperature superconductors in superhydrides stabilized under high pressure. Matter and Radiation at Extremes, 2020, 5, .	3.9	37
32	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
33	A hypervalent and cubically coordinated molecular phase of IF₈predicted at high pressure. Chemical Science, 2019, 10, 2543-2550.	7.4	36
34	Stable Lithium Argon compounds under high pressure. Scientific Reports, 2015, 5, 16675.	3.3	34
35	JAMIP: an artificial-intelligence aided data-driven infrastructure for computational materials informatics. Science Bulletin, 2021, 66, 1973-1985.	9.0	32
36	Construction of crystal structure prototype database: methods and applications. Journal of Physics Condensed Matter, 2017, 29, 165901.	1.8	31

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37	X-ray diffraction data-assisted structure searches. Computer Physics Communications, 2017, 213, 40-45.	7.5	30
38	Anatase (101)-like Structural Model Revealed for Metastable Rutile TiO₂(011) Surface. ACS Applied Materials & Interfaces, 2017, 9, 7891-7896.	8.0	29
39	Highly Efficient Selective Benzylation of Carbohydrates Catalyzed by Iron(III) with Silver Oxide and Bromide Anion as Coâ€catalysts. ChemCatChem, 2017, 9, 950-953.	3.7	29
40	The CALYPSO methodology for structure prediction*. Chinese Physics B, 2019, 28, 106105.	1.4	28
41	Study of Pickering emulsion stabilized by sulfonated cellulose nanowhiskers extracted from sisal fiber. Colloid and Polymer Science, 2015, 293, 963-974.	2.1	27
42	An inexpensive catalyst, Fe(acac)₃, for regio/site-selective acylation of diols and carbohydrates containing a 1,2-cis-diol. Green Chemistry, 2018, 20, 1987-1991.	9.0	27
43	Identifying the Ground-State NP Sheet through a Global Structure Search in Two-Dimensional Space and Its Promising High-Efficiency Photovoltaic Properties. , 2019, 1, 375-382.		26
44	Exotic Hydrogen Bonding in Compressed Ammonia Hydrides. Journal of Physical Chemistry Letters, 2019, 10, 2761-2766.	4.6	25
45	Effects of manganese doping on the structure evolution of small-sized boron clusters. Journal of Physics Condensed Matter, 2017, 29, 265401.	1.8	23
46	Large-scale ab initio simulations for periodic system. Computer Physics Communications, 2018, 233, 78-83.	7.5	23
47	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
48	Preparation and characterization of epoxy nanocomposites containing surfaceâ€modified graphene oxide. Journal of Applied Polymer Science, 2014, 131, .	2.6	22
49	The exotically stoichiometric compounds in Alâ€“S system under high pressure. Npj Computational Materials, 2020, 6, .	8.7	21
50	A One-Pot Method for Removal of Thioacetyl Group via Desulfurization under Ultraviolet Light To Synthesize Deoxyglycosides. Organic Letters, 2019, 21, 5903-5906.	4.6	20
51	Pressure-stabilized divalent ozonide CaO3 and its impact on Earthâ€™s oxygen cycles. Nature Communications, 2020, 11, 4702.	12.8	20
52	Structure and superconductivity in compressed Li-Si-H compounds: Density functional theory calculations. Physical Review B, 2020, 102, .	3.2	20
53	Nonlocal kinetic energy density functionals for isolated systems obtained via local density approximation kernels. Physical Review B, 2020, 101, .	3.2	20
54	Impact of organic molecule rotation on the optoelectronic properties of hybrid halide perovskites. Physical Review Materials, 2019, 3, .	2.4	20

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55	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
56	Regio/Site-Selective Benzoylation of Carbohydrates by Catalytic Amounts of FeCl₃. ACS Omega, 2018, 3, 17717-17723.	3.5	18
57	Structure evolution of chromium-doped boron clusters: toward the formation of endohedral boron cages. RSC Advances, 2019, 9, 2870-2876.	3.6	18
58	Interactive Genetic Algorithm Oriented toward the Novel Design of Traditional Patterns. Information (Switzerland), 2019, 10, 36.	2.9	17
59	Regioselective Sulfonylation/Acylation of Carbohydrates Catalyzed by FeCl₃ Combined with Benzoyltrifluoroacetone and Its Mechanism Study. Journal of Organic Chemistry, 2020, 85, 3307-3319.	3.2	17
60	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
61	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
62	Phase diagram and physical properties of iridium tetraboride from first principles. Physical Chemistry Chemical Physics, 2016, 18, 12569-12575.	2.8	15
63	Machine learning metadynamics simulation of reconstructive phase transition. Physical Review B, 2021, 103, .	3.2	15
64	Using DMF as Both a Catalyst and Cosolvent for the Regioselective Silylation of Polyols and Diols. European Journal of Organic Chemistry, 2019, 2019, 6383-6395.	2.4	14
65	Theoretical study of electronic and mechanical properties of Fe₂B. RSC Advances, 2016, 6, 73576-73580.	3.6	13
66	Novel structures of oxygen adsorbed on a Zr(0001) surface predicted from first principles. Applied Surface Science, 2017, 393, 422-427.	6.1	13
67	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
68	An automated predictor for identifying transition states in solids. Npj Computational Materials, 2020, 6, .	8.7	12
69	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
70	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
71	Computational Design of Mixed-Valence Tin Sulfides as Solar Absorbers. ACS Applied Materials & Interfaces, 2019, 11, 24867-24875.	8.0	11
72	Unscented Transformation-Based Multi-Robot Collaborative Self-Localization and Distributed Target Tracking. Applied Sciences (Switzerland), 2019, 9, 903.	2.5	11

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73	Stannous chloride as a low toxicity and extremely cheap catalyst for regio-/site-selective acylation with unusually broad substrate scope. Green Chemistry, 2020, 22, 6936-6942.	9.0	11
74	Structure search of two-dimensional systems using CALYPSO methodology. Frontiers of Physics, 2022, 17, 1.	5.0	11
75	Dynamic mechanical properties of sisal fiber cellulose microcrystalline/unsaturated polyester inâ€situ composites. Polymers for Advanced Technologies, 2015, 26, 1351-1355.	3.2	10
76	Decomposition and Recombination of Binary Interalkali Na₂K at High Pressures. Journal of Physical Chemistry Letters, 2019, 10, 3006-3012.	4.6	10
77	Regio/site-selective alkylation of substrates containing a cis-, 1,2- or 1,3-diol with ferric chloride and dipivaloylmethane as the catalytic system. Green Chemistry, 2020, 22, 1139-1144.	9.0	9
78	Lowest-energy structural and electronic properties of Cu Zr13â^' (nÂ=Â3â€“10) clusters in metallic glasses via CALYPSO search and density functional theory calculations. Journal of Molecular Liquids, 2021, 343, 117603.	4.9	9
79	Fabrication and Thermal Property of Polyhedral Oligomeric Silsesquioxane (POSS)/Microcrystalline Cellulose (MCC) Hybrids. Journal of Carbohydrate Chemistry, 2014, 33, 86-103.	1.1	8
80	Ground-State Crystal Structure of Strontium Peroxide Predicted from First Principles. Inorganic Chemistry, 2017, 56, 7545-7549.	4.0	7
81	A database assisted protein structure prediction method via a swarm intelligence algorithm. RSC Advances, 2017, 7, 39869-39876.	3.6	7
82	Ironâ€“magnesium compounds under high pressure. New Journal of Chemistry, 2019, 43, 17403-17407.	2.8	7
83	Synthesis and antitumor activity evaluation of a novel series of camptothecin analogs. Journal of Asian Natural Products Research, 2013, 15, 867-874.	1.4	6
84	Preparation, Characterization, and Properties of In Situ Formed Graphene Oxide/Phenol Formaldehyde Nanocomposites. Journal of Nanomaterials, 2013, 2013, 1-6.	2.7	6
85	CALYPSO Method for Structure Prediction and Its Applications to Materials Discovery. , 2019, , 1-28.		6
86	High-pressure polymorphs of LiPN2: A first-principles study. Frontiers of Physics, 2018, 13, 1.	5.0	5
87	Pressure-stabilized high-energy-density material YN₁₀. Journal of Physics Condensed Matter, 2022, 34, 135403.	1.8	5
88	Superior Mechanical Properties of GaAs Driven by Lattice Nanotwinning. Chinese Physics Letters, 2021, 38, 046201.	3.3	4
89	SnCl ₂ â€Catalyzed Acetalation/Selective Benzoylation Sequence for the Synthesis of Orthogonally Protected Glycosyl Acceptors. European Journal of Organic Chemistry, 0, , .	2.4	4
90	Preparation, Morphology, and Structure of Thermotropic Liquid Crystalline Polyester-imide/Phenol-formaldehyde Resin Blends. Journal of Macromolecular Science - Pure and Applied Chemistry, 2012, 49, 378-384.	2.2	3

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91	High-pressure modulated structures in beryllium chalcogenides. Physical Review B, 2019, 100, .	3.2	3
92	Prediction of a novel high-pressure phase of hydrogen peroxide. Physical Review B, 2020, 101, .	3.2	3
93	CALYPSO Method for Structure Prediction and Its Applications to Materials Discovery. , 2020, , 2729-2756.		3
94	Ti-fraction-induced electronic and magnetic transformations in titanium oxide films. Journal of Chemical Physics, 2019, 150, 154704.	3.0	2
95	Research on the Quantitative Method of Cognitive Loading in a Virtual Reality System. Information (Switzerland), 2019, 10, 170.	2.9	2
96	Construction and application of an ergonomic simulation optimization method driven by a posture load regulatory network. Simulation, 2020, 96, 623-637.	1.8	2
97	Stability of Ca(OH)2 at Earth's deep lower mantle conditions. Physical Review B, 2021, 104, .	3.2	2
98	Synthesis of calcium polysulfides at high pressures. Physical Review B, 2021, 104, .	3.2	2
99	Effects of preparation methods on mechanical and tribological properties of SFCM/UP composites. Polymers for Advanced Technologies, 2015, 26, 1306-1311.	3.2	1
100	Pressure-induced formation of bulk Ge-Sn compounds with high concentration of Sn. Solid State Communications, 2019, 293, 48-52.	1.9	1
101	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
102	Inorganic Crystal Structure Prototype Database Based on Unsupervised Learning of Local Atomic Environments. Journal of Physical Chemistry A, 0, , .	2.5	1
103	Pressure-induced phase transition of zinc nitride chlorine. Computational Materials Science, 2015, 106, 175-179.	3.0	0
104	Preparation and Electrocatalytic Activity of Nanophase WC-Co Composite Powder and WC Powder with Spherical Shell Structure. Materials Science Forum, 0, 816, 694-698.	0.3	0
105	Two-Dimensional TeB Structures with Anisotropic Carrier Mobility and Tunable Bandgap. Molecules, 2021, 26, 6404.	3.8	0
106	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