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	Structure search of two-dimensional systems using CALYPSO methodology. Frontiers of Physics, 2022, 17, 1.	5.0	11
2	Pressure-stabilized high-energy-density material YN₁₀. Journal of Physics Condensed Matter, 2022, 34, 135403.	1.8	5
3	A symmetry-orientated divide-and-conquer method for crystal structure prediction. Journal of Chemical Physics, 2022, 156, 014105.	3.0	40
4	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
5	Superconducting <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
6	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
7	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
8	Machine learning metadynamics simulation of reconstructive phase transition. Physical Review B, 2021, 103, .	3.2	15
9	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
10	Superior Mechanical Properties of GaAs Driven by Lattice Nanotwinning. Chinese Physics Letters, 2021, 38, 046201.	3.3	4
11	Stability of Ca(OH)2 at Earth's deep lower mantle conditions. Physical Review B, 2021, 104, .	3.2	2
12	Synthesis of calcium polysulfides at high pressures. Physical Review B, 2021, 104, .	3.2	2
13	JAMIP: an artificial-intelligence aided data-driven infrastructure for computational materials informatics. Science Bulletin, 2021, 66, 1973-1985.	9.0	32
14	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
15	Two-Dimensional TeB Structures with Anisotropic Carrier Mobility and Tunable Bandgap. Molecules, 2021, 26, 6404.	3.8	0
16	Theory-orientated discovery of high-temperature superconductors in superhydrides stabilized under high pressure. Matter and Radiation at Extremes, 2020, 5, .	3.9	37
17	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
18	Pressure-stabilized divalent ozonide CaO3 and its impact on Earthâ€™s oxygen cycles. Nature Communications, 2020, 11, 4702.	12.8	20

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19	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
20	Structure and superconductivity in compressed Li-Si-H compounds: Density functional theory calculations. Physical Review B, 2020, 102, .	3.2	20
21	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
22	Construction and application of an ergonomic simulation optimization method driven by a posture load regulatory network. Simulation, 2020, 96, 623-637.	1.8	2
23	Nonlocal kinetic energy density functionals for isolated systems obtained via local density approximation kernels. Physical Review B, 2020, 101, .	3.2	20
24	An automated predictor for identifying transition states in solids. Npj Computational Materials, 2020, 6, .	8.7	12
25	The exotically stoichiometric compounds in Alâ€“S system under high pressure. Npj Computational Materials, 2020, 6, .	8.7	21
26	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
27	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
28	Prediction of a novel high-pressure phase of hydrogen peroxide. Physical Review B, 2020, 101, .	3.2	3
29	CALYPSO Method for Structure Prediction and Its Applications to Materials Discovery. , 2020, , 2729-2756.		3
30	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
31	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
32	High-pressure modulated structures in beryllium chalcogenides. Physical Review B, 2019, 100, .	3.2	3
33	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
34	The CALYPSO methodology for structure prediction*. Chinese Physics B, 2019, 28, 106105.	1.4	28
35	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
36	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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37	Structure evolution of chromium-doped boron clusters: toward the formation of endohedral boron cages. RSC Advances, 2019, 9, 2870-2876.	3.6	18
38	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
39	Decomposition and Recombination of Binary Interalkali Na₂K at High Pressures. Journal of Physical Chemistry Letters, 2019, 10, 3006-3012.	4.6	10
40	Exotic Hydrogen Bonding in Compressed Ammonia Hydrides. Journal of Physical Chemistry Letters, 2019, 10, 2761-2766.	4.6	25
41	Ti-fraction-induced electronic and magnetic transformations in titanium oxide films. Journal of Chemical Physics, 2019, 150, 154704.	3.0	2
42	Research on the Quantitative Method of Cognitive Loading in a Virtual Reality System. Information (Switzerland), 2019, 10, 170.	2.9	2
43	Computational Design of Mixed-Valence Tin Sulfides as Solar Absorbers. ACS Applied Materials & Interfaces, 2019, 11, 24867-24875.	8.0	11
44	Unscented Transformation-Based Multi-Robot Collaborative Self-Localization and Distributed Target Tracking. Applied Sciences (Switzerland), 2019, 9, 903.	2.5	11
45	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
46	Interactive Genetic Algorithm Oriented toward the Novel Design of Traditional Patterns. Information (Switzerland), 2019, 10, 36.	2.9	17
47	Interface structure prediction via CALYPSO method. Science Bulletin, 2019, 64, 301-309.	9.0	219
48	Pressure-induced formation of bulk Ge-Sn compounds with high concentration of Sn. Solid State Communications, 2019, 293, 48-52.	1.9	1
49	Ironâ€“magnesium compounds under high pressure. New Journal of Chemistry, 2019, 43, 17403-17407.	2.8	7
50	CALYPSO Method for Structure Prediction and Its Applications to Materials Discovery. , 2019, , 1-28.		6
51	Impact of organic molecule rotation on the optoelectronic properties of hybrid halide perovskites. Physical Review Materials, 2019, 3, .	2.4	20
52	High-pressure polymorphs of LiPN2: A first-principles study. Frontiers of Physics, 2018, 13, 1.	5.0	5
53	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
54	Accelerating CALYPSO structure prediction by data-driven learning of a potential energy surface. Faraday Discussions, 2018, 211, 31-43.	3.2	76

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55	Perovskite Solar Absorbers: Materials by Design. Small Methods, 2018, 2, 1700316.	8.6	95
56	Regio/Site-Selective Benzoylation of Carbohydrates by Catalytic Amounts of FeCl₃. ACS Omega, 2018, 3, 17717-17723.	3.5	18
57	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> Stabilized at Deep-Earth Conditions. Physical Review Letters, 2018, 121, 255703.	7.8	68
58	Direct-gap semiconducting tri-layer silicene with 29% photovoltaic efficiency. Nano Energy, 2018, 51, 489-495.	16.0	46
59	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
60	Large-scale ab initio simulations for periodic system. Computer Physics Communications, 2018, 233, 78-83.	7.5	23
61	Materials discovery at high pressures. Nature Reviews Materials, 2017, 2, .	48.7	427
62	Anatase (101)-like Structural Model Revealed for Metastable Rutile TiO₂(011) Surface. ACS Applied Materials & Interfaces, 2017, 9, 7891-7896.	8.0	29
63	Effects of manganese doping on the structure evolution of small-sized boron clusters. Journal of Physics Condensed Matter, 2017, 29, 265401.	1.8	23
64	Ground-State Crystal Structure of Strontium Peroxide Predicted from First Principles. Inorganic Chemistry, 2017, 56, 7545-7549.	4.0	7
65	Construction of crystal structure prototype database: methods and applications. Journal of Physics Condensed Matter, 2017, 29, 165901.	1.8	31
66	X-ray diffraction data-assisted structure searches. Computer Physics Communications, 2017, 213, 40-45.	7.5	30
67	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
68	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
69	A two-dimensional TiB₄monolayer exhibits planar octacoordinate Ti. Nanoscale, 2017, 9, 17983-17990.	5.6	50
70	A database assisted protein structure prediction method via a swarm intelligence algorithm. RSC Advances, 2017, 7, 39869-39876.	3.6	7
71	Novel structures of oxygen adsorbed on a Zr(0001) surface predicted from first principles. Applied Surface Science, 2017, 393, 422-427.	6.1	13
72	Phase diagram and physical properties of iridium tetraboride from first principles. Physical Chemistry Chemical Physics, 2016, 18, 12569-12575.	2.8	15

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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	Theoretical study of electronic and mechanical properties of Fe₂B. RSC Advances, 2016, 6, 73576-73580.	3.6	13
75	CALYPSO structure prediction method and its wide application. Computational Materials Science, 2016, 112, 406-415.	3.0	138
76	Understanding the structural transformation, stability of medium-sized neutral and charged silicon clusters. Scientific Reports, 2015, 5, 15951.	3.3	52
77	Stable Lithium Argon compounds under high pressure. Scientific Reports, 2015, 5, 16675.	3.3	34
78	Dynamic mechanical properties of sisal fiber cellulose microcrystalline/unsaturated polyester inâ€situ composites. Polymers for Advanced Technologies, 2015, 26, 1351-1355.	3.2	10
79	Effects of preparation methods on mechanical and tribological properties of SFCM/UP composites. Polymers for Advanced Technologies, 2015, 26, 1306-1311.	3.2	1
80	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
81	Study of Pickering emulsion stabilized by sulfonated cellulose nanowhiskers extracted from sisal fiber. Colloid and Polymer Science, 2015, 293, 963-974.	2.1	27
82	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
83	Pressure-induced phase transition of zinc nitride chlorine. Computational Materials Science, 2015, 106, 175-179.	3.0	0
84	Materials discovery via CALYPSO methodology. Journal of Physics Condensed Matter, 2015, 27, 203203.	1.8	93
85	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
86	Stabilization of fullerene-like boron cages by transition metal encapsulation. Nanoscale, 2015, 7, 10482-10489.	5.6	72
87	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
88	Fabrication and Thermal Property of Polyhedral Oligomeric Silsesquioxane (POSS)/Microcrystalline Cellulose (MCC) Hybrids. Journal of Carbohydrate Chemistry, 2014, 33, 86-103.	1.1	8
89	B₃₈: an all-boron fullerene analogue. Nanoscale, 2014, 6, 11692-11696.	5.6	153
90	Preparation and characterization of epoxy nanocomposites containing surfaceâ€modified graphene oxide. Journal of Applied Polymer Science, 2014, 131, .	2.6	22

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91	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
92	First-principles structural design of superhard materials. Journal of Chemical Physics, 2013, 138, 114101.	3.0	176
93	Preparation, Characterization, and Properties of In Situ Formed Graphene Oxide/Phenol Formaldehyde Nanocomposites. Journal of Nanomaterials, 2013, 2013, 1-6.	2.7	6
94	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
95	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
96	Cagelike Diamondoid Nitrogen at High Pressures. Physical Review Letters, 2012, 109, 175502.	7.8	176
97	Particle-swarm structure prediction on clusters. Journal of Chemical Physics, 2012, 137, 084104.	3.0	453
98	CALYPSO: A method for crystal structure prediction. Computer Physics Communications, 2012, 183, 2063-2070.	7.5	2,085
99	Substitutional Alloy of Bi and Te at High Pressure. Physical Review Letters, 2011, 106, 145501.	7.8	363
100	High pressure partially ionic phase of water ice. Nature Communications, 2011, 2, 563.	12.8	208
101	Predicted Novel High-Pressure Phases of Lithium. Physical Review Letters, 2011, 106, 015503.	7.8	499
102	Crystal structure prediction via particle-swarm optimization. Physical Review B, 2010, 82, .	3.2	1,870
103	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
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	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
106	Inorganic Crystal Structure Prototype Database Based on Unsupervised Learning of Local Atomic Environments. Journal of Physical Chemistry A, 0, , .	2.5	1