Quan Li

List of Publications by Year
in descending order

98 papers	4,264 citations	117453 34 h-index	118652 62 g-index
100 all docs	100 docs citations	100 times ranked	3184 citing authors

#	Article	IF	Citations
1	Superhard Monoclinic Polymorph of Carbon. Physical Review Letters, 2009, 102, 175506.	2.9	480
2	Global Structural Optimization of Tungsten Borides. Physical Review Letters, 2013, 110, 136403.	2.9	253
3	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.	2.9	180
4	First-principles structural design of superhard materials. Journal of Chemical Physics, 2013, 138, 114101.	1.2	176
5	Tetragonal Allotrope of Group 14 Elements. Journal of the American Chemical Society, 2012, 134, 12362-12365.	6.6	170
6	CALYPSO structure prediction method and its wide application. Computational Materials Science, 2016, 112, 406-415.	1.4	138
7	Extraordinary Indentation Strain Stiffening Produces Superhard Tungsten Nitrides. Physical Review Letters, 2017, 119, 115503.	2.9	129
8	Predicted Lithiumâ€“Boron Compounds under High Pressure. Journal of the American Chemical Society, 2012, 134, 18599-18605.	6.6	113
9	A novel low compressible and superhard carbon nitride: Body-centered tetragonal CN2. Physical Chemistry Chemical Physics, 2012, 14, 13081.	1.3	108
10	Anomalous Stress Response of Ultrahard<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>WB</mml:mi></mml:mrow><mml:mrow><mml:mi>n</mml:mi></mml:mrow> Physical Review Letters, 2015, 115, 185502.	2.9	107
11	Elucidating Stressâ€“Strain Relations of ZrB₁₂ from First-Principles Studies. Journal of Physical Chemistry Letters, 2020, 11, 9165-9170.	2.1	97
12	High-pressure strengthening in ultrafine-grained metals. Nature, 2020, 579, 67-72.	13.7	96
13	Materials discovery via CALYPSO methodology. Journal of Physics Condensed Matter, 2015, 27, 203203.	0.7	93
14	Pressure-induced phase transitions and metallization in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>VO</mml:mi><mml:mn>2</mml:mn></mml:msub> Physical Review B, 2015, 91, .	1.1	82
15	Exploring Hardness and the Distorted sp² Hybridization of Bâ€“B Bonds in WB₃. Chemistry of Materials, 2014, 26, 5297-5302.	3.2	80
16	2D Materials and Heterostructures at Extreme Pressure. Advanced Science, 2020, 7, 2002697.	5.6	68
17	Superhard and superconducting structures of BC5. Journal of Applied Physics, 2010, 108, .	1.1	66
18	Ab initio prediction of superconductivity in molecular metallic hydrogen under high pressure. Solid State Communications, 2007, 141, 610-614.	0.9	65

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19	Superconductivity in Compression-Shear Deformed Diamond. Physical Review Letters, 2020, 124, 147001.	2.9	64
20	Orthorhombic C32: a novel superhard sp3 carbon allotrope. Physical Chemistry Chemical Physics, 2013, 15, 14120.	1.3	62
21	Superhard and superconductive polymorphs of diamond-like BC3. Physics Letters, Section A: General, Atomic and Solid State Physics, 2011, 375, 771-774.	0.9	59
22	Superconductivity of lithium-doped hydrogen under high pressure. Acta Crystallographica Section C, Structural Chemistry, 2014, 70, 104-111.	0.2	59
23	Ultra-incompressible phases of tungsten dinitride predicted from first principles. Physical Review B, 2009, 79, .	1.1	58
24	Rhombohedral superhard structure of BC2N. Journal of Applied Physics, 2009, 105, 053514.	1.1	54
25	Enhanced Vickers hardness by quasi-3D boron network in MoB2. RSC Advances, 2013, 3, 18317.	1.7	53
26	Smooth Flow in Diamond: Atomistic Ductility and Electronic Conductivity. Physical Review Letters, 2019, 123, 195504.	2.9	50
27	Twofold Coordinated Ground-State and Eightfold High-Pressure Phases of Heavy Transition Metal Nitrides MN₂ (M = Os, Ir, Ru, and Rh). Inorganic Chemistry, 2009, 48, 9904-9909.	1.9	47
28	Structural and electronic properties of sodium azide at high pressure: A first principles study. Solid State Communications, 2013, 161, 13-18.	0.9	47
29	Planar NiC₃ as a reversible anode material with high storage capacity for lithium-ion and sodium-ion batteries. Journal of Materials Chemistry A, 2019, 7, 13356-13363.	5.2	47
30	Predicting new superhard phases. Journal of Superhard Materials, 2010, 32, 192-204.	0.5	46
31	Ultrahigh capacity 2D anode materials for lithium/sodium-ion batteries: an entirely planar B₇P₂ monolayer with suitable pore size and distribution. Journal of Materials Chemistry A, 2020, 8, 10301-10309.	5.2	44
32	Superhard polymorphs of diamond-like. Solid State Communications, 2011, 151, 716-719.	0.9	38
33	B ₂ CO: A potential superhard material in the B-C-O system. Europhysics Letters, 2011, 95, 66006.	0.7	37
34	Unraveling Convoluted Structural Transitions in SnTe at High Pressure. Journal of Physical Chemistry C, 2013, 117, 5352-5357.	1.5	36
35	Orthorhombic BN: A novel superhard boron nitride allotrope. Physics Letters, Section A: General, Atomic and Solid State Physics, 2014, 378, 741-744.	0.9	33
36	Pressure-Induced Superconductivity in SnTe: A First-Principles Study. Journal of Physical Chemistry C, 2013, 117, 12266-12271.	1.5	31

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37	Construction of crystal structure prototype database: methods and applications. Journal of Physics Condensed Matter, 2017, 29, 165901.	0.7	31
38	Oxygen vacancies dependent phase transition of Y2O3 films. Applied Surface Science, 2017, 410, 470-478.	3.1	31
39	Anatase (101)-like Structural Model Revealed for Metastable Rutile TiO₂(011) Surface. ACS Applied Materials & Interfaces, 2017, 9, 7891-7896.	4.0	29
40	TMC (TM = Co, Ni, and Cu) monolayers with planar pentacoordinate carbon and their potential applications. Journal of Materials Chemistry C, 2019, 7, 6406-6413.	2.7	29
41	Xenon iron oxides predicted as potential Xe hosts in Earthâ€™s lower mantle. Nature Communications, 2020, 11, 5227.	5.8	27
42	Superconductivity in HfTe5 across weak to strong topological insulator transition induced via pressures. Scientific Reports, 2017, 7, 44367.	1.6	25
43	Exotic Hydrogen Bonding in Compressed Ammonia Hydrides. Journal of Physical Chemistry Letters, 2019, 10, 2761-2766.	2.1	25
44	Unravelling the structure and strength of the highest boride of tungsten <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">WB</mml:mi><mml:mrow><mml:mn>4.2</mml:mn></mml:mrow></mml:msub></mml:math>. Physical Review B, 2019, 100, .	1.1	25
45	Structural metatransition of energetically tangled crystalline phases. Physical Chemistry Chemical Physics, 2017, 19, 4560-4566.	1.3	23
46	High-Pressure Evolution of Unexpected Chemical Bonding and Promising Superconducting Properties of YB₆. Journal of Physical Chemistry C, 2018, 122, 27820-27828.	1.5	23
47	Pressure-induced phase transition, metallization and superconductivity in ZrS₂. Physical Chemistry Chemical Physics, 2018, 20, 23656-23663.	1.3	23
48	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.	3.3	23
49	Orientationally disordered <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mtext>H</mml:mtext><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math> the high-pressure van der Waals compound <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"		

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55	Superhard-driven search of the covalent network in the B₃NO system. RSC Advances, 2015, 5, 35882-35887.	1.7	18
56	Pressure-induced cation-cation bonding in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi mathvariant="normal">V</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math>. Physical Review B, 2015, 92, .	1.1	17
57	Investigations on structural determination of semi-transition-metal borides. Physical Chemistry Chemical Physics, 2017, 19, 31592-31598.	1.3	17
58	Superconductivity in Shear Strained Semiconductors. Chinese Physics Letters, 2021, 38, 086301.	1.3	17
59	Superhard phases of B2O: An isoelectronic compound of diamond. Diamond and Related Materials, 2011, 20, 501-504.	1.8	16
60	Crystal and electronic structures of superhard B2CN : An ab initio study. Solid State Communications, 2012, 152, 71-75.	0.9	16
61	Pressure-Driven Enhancement of Topological Insulating State in Tin Telluride. Journal of Physical Chemistry C, 2013, 117, 8437-8442.	1.5	16
62	Exploring High-Pressure Structures of N₂CO. Journal of Physical Chemistry C, 2014, 118, 27252-27257.	1.5	16
63	The effects of pressure on the electronic, transport and dynamical properties of AuX₂(X =) Tj ETQq1 1 0.784314 rgBT /O	0.7	15
64	Phase-transition mechanism of h-BN w-BN from first principles. Solid State Communications, 2009, 149, 843-846.	0.9	15
65	High-pressure phase transition of cesium chloride and cesium bromide. Physical Chemistry Chemical Physics, 2014, 16, 17924-17929.	1.3	15
66	Crystal Structures and Electronic Properties of Cesium Xenides at High Pressures. Journal of Physical Chemistry C, 2015, 119, 24996-25002.	1.5	15
67	Strain-induced modulations of electronic structure and electronâ€“phonon coupling in dense H₃S. Physical Chemistry Chemical Physics, 2018, 20, 5952-5957.	1.3	15
68	Synthesis and characterization of WB2-WB3-B4C hard composites. International Journal of Refractory Metals and Hard Materials, 2019, 82, 268-272.	1.7	15
69	Machine learning metadynamics simulation of reconstructive phase transition. Physical Review B, 2021, 103, .	1.1	15
70	Pronounced Enhancement of Superconductivity in ZrN via Strain Engineering. Journal of Physical Chemistry Letters, 2021, 12, 1985-1990.	2.1	15
71	All Boron Atoms in a ScB₁₂ Monolayer Contribute to the Hydrogen Evolution Reaction. Journal of Physical Chemistry C, 2020, 124, 23221-23229.	1.5	14
72	Stress-induced high- T _c superconductivity in solid molecular hydrogen. Proceedings of the National Academy of Sciences of the United States of America, 2022, 119, .	3.3	14

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73	Novel superhard polymorphs of Be3N2 predicted by first-principles. Computational Materials Science, 2010, 49, S76-S79.	1.4	13
74	Hypervalent Iodine with Linear Chain at High Pressure. Scientific Reports, 2015, 5, 14393.	1.6	13
75	Theoretical study of electronic and mechanical properties of Fe₂B. RSC Advances, 2016, 6, 73576-73580.	1.7	13
76	Experimental Observation of the High Pressure Induced Substitutional Solid Solution and Phase Transformation in Sb2S3. Scientific Reports, 2018, 8, 14795.	1.6	13
77	High pressureâ€“low temperature phase diagram of barium: Simplicity versus complexity. Applied Physics Letters, 2015, 107, .	1.5	9
78	Pressure Driven Enhancement of Ideal Shear Strength in bc8-Carbon and Diamond. Journal of Physical Chemistry C, 2017, 121, 26457-26464.	1.5	9
79	Effect of pressure on the structural, electronic and mechanical properties of ultraincompressible W₂B. RSC Advances, 2018, 8, 35664-35671.	1.7	9
80	First-principles study of high-pressure phase stability and superconductivity of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Bi</mml:mi><mml:mn>4</mml:mn></mml:n mathvariant="normal">I</mml:mi><mml:mn>4</mml:mn></mml:msub></mml:mrow></mml:math>. Physical Review B, 2019, 100, .	1.1	9
81	Atomistic Mechanisms for Contrasting Stressâ€“Strain Relations of B₁₃CN and B₁₃C₂. Journal of Physical Chemistry Letters, 2020, 11, 10454-10462.	2.1	9
82	Low-density superhard materials: computational study of Li-inserted B-substituted closo-carboranes LiBC₁₁ and Li₂B₂C₁₀. RSC Advances, 2016, 6, 52695-52699.	1.7	8
83	Globally stable structures of Li_xZn (x = 1â€“4) compounds at high pressures. Physical Chemistry Chemical Physics, 2016, 18, 4437-4443.	1.3	8
84	Toughening a superstrong carbon crystal: Sequential bond-breaking mechanisms. Physical Review B, 2020, 102, .	1.1	8
85	Computational discovery and characterization of new B₂O phases. Physical Chemistry Chemical Physics, 2019, 21, 2499-2506.	1.3	7
86	Pressure-Induced Evolution of Crystal and Electronic Structure of Ammonia Borane. Journal of Physical Chemistry Letters, 2021, 12, 2036-2043.	2.1	7
87	CALYPSO Method for Structure Prediction and Its Applications to Materials Discovery. , 2019, , 1-28.		6
88	Exploring the metallic phase of N2O under high pressure. RSC Advances, 2015, 5, 65745-65749.	1.7	5
89	Theoretical design of diamondlike superhard structures at high pressure. Chinese Physics B, 2016, 25, 076103.	0.7	5
90	New Icosahedra-based B4N phases by particle swarm optimization. Journal of Alloys and Compounds, 2021, 854, 157255.	2.8	5

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91	Mechanical properties and superconductivity in two-dimensional B2O under extreme strain. Physical Chemistry Chemical Physics, 2019, 21, 25859-25864.	1.3	4
92	Electron deficiency but semiconductive diamond-like B₂CN originated from three-center bonds. Physical Chemistry Chemical Physics, 2021, 23, 3087-3092.	1.3	4
93	Superior Mechanical Properties of GaAs Driven by Lattice Nanotwinning. Chinese Physics Letters, 2021, 38, 046201.	1.3	4
94	High-pressure polymorphs of Li2BeH4predicted by first-principles calculations. Journal of Physics Condensed Matter, 2009, 21, 385405.	0.7	3
95	CALYPSO Method for Structure Prediction and Its Applications to Materials Discovery. , 2020, , 2729-2756.		3
96	Prediction of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">Li</mml:mi><mml:mi>n</mml:mi></mml:msub><mml:mtext>Cd</mml:mtext></mml:math> compounds with unusual stoichiometry and valence states. Physical Review Materials, 2020, 4, .	0.9	3
97	Ab initio simulation of core-hole effects on the X-ray absorption near edge structure of GaP. Physica B: Condensed Matter, 2009, 404, 1643-1647.	1.3	2
98	Stability and mechanical properties of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">W</mml:mi><mml:mrow><mml:mn>1</mml:mn><mml:mo>â^'</mml:mo><mml:mi>x</mml:mi></mml:mrow><mml:mi mathvariant="normal">Mo</mml:mi><mml:mi>x</mml:mi></mml:msub><mml:msub><mml:mi mathvariant="normal">B</mml:mi><mml:mrow><mml:mn>4.2</mml:mn></mml:mrow></mml:msub></mml:math>		