Quan Li

List of Publications by Year
in descending order

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98 papers	4,264 citations	117571 34 h-index	118793 62 g-index
100 all docs	100 docs citations	100 times ranked	3184 citing authors

#	Article	IF	Citations
1	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
2	New Icosahedra-based B4N phases by particle swarm optimization. Journal of Alloys and Compounds, 2021, 854, 157255.	2.8	5
3	Electron deficiency but semiconductive diamond-like B₂CN originated from three-center bonds. Physical Chemistry Chemical Physics, 2021, 23, 3087-3092.	1.3	4
4	Machine learning metadynamics simulation of reconstructive phase transition. Physical Review B, 2021, 103, .	1.1	15
5	Pronounced Enhancement of Superconductivity in ZrN via Strain Engineering. Journal of Physical Chemistry Letters, 2021, 12, 1985-1990.	2.1	15
6	Pressure-Induced Evolution of Crystal and Electronic Structure of Ammonia Borane. Journal of Physical Chemistry Letters, 2021, 12, 2036-2043.	2.1	7
7	Superior Mechanical Properties of GaAs Driven by Lattice Nanotwinning. Chinese Physics Letters, 2021, 38, 046201.	1.3	4
8	Superconductivity in Shear Strained Semiconductors. Chinese Physics Letters, 2021, 38, 086301.	1.3	17
9	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>âˆ’</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>		

#	Article	IF	Citations
19	Superconductivity in Compression-Shear Deformed Diamond. Physical Review Letters, 2020, 124, 147001.	2.9	64
20	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
21	CALYPSO Method for Structure Prediction and Its Applications to Materials Discovery. , 2020, , 2729-2756.		3
22	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
23	Smooth Flow in Diamond: Atomistic Ductility and Electronic Conductivity. Physical Review Letters, 2019, 123, 195504.	2.9	50
24	Computational discovery and characterization of new B₂O phases. Physical Chemistry Chemical Physics, 2019, 21, 2499-2506.	1.3	7
25	Synthesis and characterization of WB2-WB3-B4C hard composites. International Journal of Refractory Metals and Hard Materials, 2019, 82, 268-272.	1.7	15
26	Exotic Hydrogen Bonding in Compressed Ammonia Hydrides. Journal of Physical Chemistry Letters, 2019, 10, 2761-2766.	2.1	25
27	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
28	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
29	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
30	Mechanical properties and superconductivity in two-dimensional B2O under extreme strain. Physical Chemistry Chemical Physics, 2019, 21, 25859-25864.	1.3	4
31	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:mn></mm mathvariant="normal">I</mml:mi><mml:mn>4</mml:mn></mml:msub></mml:mrow></mml:math>. Physical Review B, 2019, 100, .	1.1	9
32	CALYPSO Method for Structure Prediction and Its Applications to Materials Discovery. , 2019, , 1-28.		6
33	Strain-induced modulations of electronic structure and electronâ€"phonon coupling in dense H₃S. Physical Chemistry Chemical Physics, 2018, 20, 5952-5957.	1.3	15
34	Effect of pressure on the structural, electronic and mechanical properties of ultraincompressible W₂B. RSC Advances, 2018, 8, 35664-35671.	1.7	9
35	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
36	Experimental Observation of the High Pressure Induced Substitutional Solid Solution and Phase Transformation in Sb2S3. Scientific Reports, 2018, 8, 14795.	1.6	13

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37	Pressure-induced phase transition, metallization and superconductivity in ZrS₂. Physical Chemistry Chemical Physics, 2018, 20, 23656-23663.	1.3	23
38	Structural metatransition of energetically tangled crystalline phases. Physical Chemistry Chemical Physics, 2017, 19, 4560-4566.	1.3	23
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	Construction of crystal structure prototype database: methods and applications. Journal of Physics Condensed Matter, 2017, 29, 165901.	0.7	31
41	Oxygen vacancies dependent phase transition of Y2O3 films. Applied Surface Science, 2017, 410, 470-478.	3.1	31
42	Extraordinary Indentation Strain Stiffening Produces Superhard Tungsten Nitrides. Physical Review Letters, 2017, 119, 115503.	2.9	129
43	Superconductivity in HfTe5 across weak to strong topological insulator transition induced via pressures. Scientific Reports, 2017, 7, 44367.	1.6	25
44	Pressure Driven Enhancement of Ideal Shear Strength in bc8-Carbon and Diamond. Journal of Physical Chemistry C, 2017, 121, 26457-26464.	1.5	9
45	Investigations on structural determination of semi-transition-metal borides. Physical Chemistry Chemical Physics, 2017, 19, 31592-31598.	1.3	17
46	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
47	Theoretical study of electronic and mechanical properties of Fe₂B. RSC Advances, 2016, 6, 73576-73580.	1.7	13
48	Theoretical design of diamondlike superhard structures at high pressure. Chinese Physics B, 2016, 25, 076103.	0.7	5
49	Globally stable structures of Li_xZn (x = 1â€“4) compounds at high pressures. Physical Chemistry Chemical Physics, 2016, 18, 4437-4443.	1.3	8
50	CALYPSO structure prediction method and its wide application. Computational Materials Science, 2016, 112, 406-415.	1.4	138
51	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>.	1.1	17
52	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></mm Physical Review Letters, 2015, 115, 185502.	2.9	107
53	Hypervalent Iodine with Linear Chain at High Pressure. Scientific Reports, 2015, 5, 14393.	1.6	13
54	High pressureâ€“low temperature phase diagram of barium: Simplicity versus complexity. Applied Physics Letters, 2015, 107, .	1.5	9

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55	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
56	Exploring the metallic phase of N2O under high pressure. RSC Advances, 2015, 5, 65745-65749.	1.7	5
57	Materials discovery via CALYPSO methodology. Journal of Physics Condensed Matter, 2015, 27, 203203.	0.7	93
58	Superhard-driven search of the covalent network in the B₃NO system. RSC Advances, 2015, 5, 35882-35887.	1.7	18
59	Crystal Structures and Electronic Properties of Cesium Xenides at High Pressures. Journal of Physical Chemistry C, 2015, 119, 24996-25002.	1.5	15
60	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></mml Physical Review B, 2015, 91, .	1.1	82
61	Exploring High-Pressure Structures of N₂CO. Journal of Physical Chemistry C, 2014, 118, 27252-27257.	1.5	16
62	Crystal structure and physical properties of Mo2B: First-principle calculations. Journal of Applied Physics, 2014, 115, .	1.1	21
63	High-pressure phase transition of cesium chloride and cesium bromide. Physical Chemistry Chemical Physics, 2014, 16, 17924-17929.	1.3	15
64	Structural and Mechanical Properties of Platinum Carbide. Inorganic Chemistry, 2014, 53, 5797-5802.	1.9	19
65	Superconductivity of lithium-doped hydrogen under high pressure. Acta Crystallographica Section C, Structural Chemistry, 2014, 70, 104-111.	0.2	59
66	Exploring Hardness and the Distorted sp² Hybridization of Bâ€"B Bonds in WB₃. Chemistry of Materials, 2014, 26, 5297-5302.	3.2	80
67	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
68	Unraveling Convoluted Structural Transitions in SnTe at High Pressure. Journal of Physical Chemistry C, 2013, 117, 5352-5357.	1.5	36
69	Orthorhombic C32: a novel superhard sp3 carbon allotrope. Physical Chemistry Chemical Physics, 2013, 15, 14120.	1.3	62
70	Enhanced Vickers hardness by quasi-3D boron network in MoB2. RSC Advances, 2013, 3, 18317.	1.7	53
71	Structural and electronic properties of sodium azide at high pressure: A first principles study. Solid State Communications, 2013, 161, 13-18.	0.9	47
72	Global Structural Optimization of Tungsten Borides. Physical Review Letters, 2013, 110, 136403.	2.9	253

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73	Pressure-Induced Superconductivity in SnTe: A First-Principles Study. Journal of Physical Chemistry C, 2013, 117, 12266-12271.	1.5	31
74	First-principles structural design of superhard materials. Journal of Chemical Physics, 2013, 138, 114101.	1.2	176
75	Pressure-Driven Enhancement of Topological Insulating State in Tin Telluride. Journal of Physical Chemistry C, 2013, 117, 8437-8442.	1.5	16
76	Direct Observation of a Pressure-Induced Precursor Lattice in Silicon. Physical Review Letters, 2012, 109, 205503.	2.9	22
77	A novel low compressible and superhard carbon nitride: Body-centered tetragonal CN2. Physical Chemistry Chemical Physics, 2012, 14, 13081.	1.3	108
78	Predicted Lithiumâ€"Boron Compounds under High Pressure. Journal of the American Chemical Society, 2012, 134, 18599-18605.	6.6	113
79	Tetragonal Allotrope of Group 14 Elements. Journal of the American Chemical Society, 2012, 134, 12362-12365.	6.6	170
80	Crystal and electronic structures of superhard B2CN : An ab initio study. Solid State Communications, 2012, 152, 71-75.	0.9	16
81	B ₂ CO: A potential superhard material in the B-C-O system. Europhysics Letters, 2011, 95, 66006.	0.7	37
82	Superhard phases of B2O: An isoelectronic compound of diamond. Diamond and Related Materials, 2011, 20, 501-504.	1.8	16
83	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
84	Superhard polymorphs of diamond-like. Solid State Communications, 2011, 151, 716-719.	0.9	38
85	Predicting new superhard phases. Journal of Superhard Materials, 2010, 32, 192-204.	0.5	46
86	Superhard and superconducting structures of BC5. Journal of Applied Physics, 2010, 108, .	1.1	66
87	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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91	Rhombohedral superhard structure of BC2N. Journal of Applied Physics, 2009, 105, 053514.	1.1	54
92	High-pressure polymorphs of Li2BeH4predicted by first-principles calculations. Journal of Physics Condensed Matter, 2009, 21, 385405.	0.7	3
93	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
94	Phase-transition mechanism of h-BN w-BN from first principles. Solid State Communications, 2009, 149, 843-846.	0.9	15
95	Superhard Monoclinic Polymorph of Carbon. Physical Review Letters, 2009, 102, 175506.	2.9	480
96	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
97	The effects of pressure on the electronic, transport and dynamical properties of AuX₂(X =) Tj ETQq1 1 0.784314 rgBT /Ove	0.7	15
98	Ab initio prediction of superconductivity in molecular metallic hydrogen under high pressure. Solid State Communications, 2007, 141, 610-614.	0.9	65