Quan Li

List of Publications by Year in Descending Order

95 papers	3,244 citations	30 h-index	55 g-index
100 ext. papers	3,783 ext. citations	5.2 avg, IF	5.34 L-index

#	Paper	IF	Citations
95	Superconductivity in Shear Strained Semiconductors. *Chinese Physics Letters*, **2021**, 38, 086301	1.8	5
94	Superior Mechanical Properties of GaAs Driven by Lattice Nanotwinning. *Chinese Physics Letters*, **2021**, 38, 046201	1.8	0
93	New Icosahedra-based B4N phases by particle swarm optimization. *Journal of Alloys and Compounds*, **2021**, 854, 157255	5.7	3
92	Electron deficiency but semiconductive diamond-like BCN originated from three-center bonds. *Physical Chemistry Chemical Physics*, **2021**, 23, 3087-3092	3.6	2
91	Machine learning metadynamics simulation of reconstructive phase transition. *Physical Review B*, **2021**, 103,	3.3	6
90	Pronounced Enhancement of Superconductivity in ZrN via Strain Engineering. *Journal of Physical Chemistry Letters*, **2021**, 12, 1985-1990	6.4	5
89	Pressure-Induced Evolution of Crystal and Electronic Structure of Ammonia Borane. *Journal of Physical Chemistry Letters*, **2021**, 12, 2036-2043	6.4	2
88	2D Materials and Heterostructures at Extreme Pressure. *Advanced Science*, **2020**, 7, 2002697	13.6	23
87	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
86	High-pressure strengthening in ultrafine-grained metals. *Nature*, **2020**, 579, 67-72	50.4	52
85	Ultralow-Friction and Ultralow-Wear TiN-Ag Solid Solution Coating in Base Oil. *Journal of Physical Chemistry Letters*, **2020**, 11, 1614-1621	6.4	8
84	Superconductivity in Compression-Shear Deformed Diamond. *Physical Review Letters*, **2020**, 124, 147001	7.4	33
83	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	13	13
82	CALYPSO Method for Structure Prediction and Its Applications to Materials Discovery **2020**, 2729-2756		1
81	Toughening a superstrong carbon crystal: Sequential bond-breaking mechanisms. *Physical Review B*, **2020**, 102,	3.3	2
80	Elucidating Stress-Strain Relations of ZrB from First-Principles Studies. *Journal of Physical Chemistry Letters*, **2020**, 11, 9165-9170	6.4	50
79	All Boron Atoms in a ScB12 Monolayer Contribute to the Hydrogen Evolution Reaction. *Journal of Physical Chemistry C*, **2020**, 124, 23221-23229	3.8	4

78	Atomistic Mechanisms for Contrasting Stress-Strain Relations of BCN and BC. *Journal of Physical Chemistry Letters*, **2020**, 11, 10454-10462	6.4	3
77	Xenon iron oxides predicted as potential Xe hosts in Earth\'s lower mantle. *Nature Communications*, **2020**, 11, 5227	17.4	6
76	Computational discovery and characterization of new BO phases. *Physical Chemistry Chemical Physics*, **2019**, 21, 2499-2506	3.6	6
75	Synthesis and characterization of WB2-WB3-B4C hard composites. *International Journal of Refractory Metals and Hard Materials*, **2019**, 82, 268-272	4.1	5
74	Exotic Hydrogen Bonding in Compressed Ammonia Hydrides. *Journal of Physical Chemistry Letters*, **2019**, 10, 2761-2766	6.4	17
73	TMC (TM = Co, Ni, and Cu) monolayers with planar pentacoordinate carbon and their potential applications. *Journal of Materials Chemistry C*, **2019**, 7, 6406-6413	7.1	21
72	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	13	23
71	Smooth Flow in Diamond: Atomistic Ductility and Electronic Conductivity. *Physical Review Letters*, **2019**, 123, 195504	7.4	27
70	Unravelling the structure and strength of the highest boride of tungsten WB4.2. *Physical Review B*, **2019**, 100,	3.3	16
69	Mechanical properties and superconductivity in two-dimensional BO under extreme strain. *Physical Chemistry Chemical Physics*, **2019**, 21, 25859-25864	3.6	4
68	First-principles study of high-pressure phase stability and superconductivity of Bi4I4. *Physical Review B*, **2019**, 100,	3.3	4
67	CALYPSO Method for Structure Prediction and Its Applications to Materials Discovery **2019**, 1-28		5
66	Strain-induced modulations of electronic structure and electron-phonon coupling in dense HS. *Physical Chemistry Chemical Physics*, **2018**, 20, 5952-5957	3.6	13
65	Pressure-induced phase transition, metallization and superconductivity in ZrS. *Physical Chemistry Chemical Physics*, **2018**, 20, 23656-23663	3.6	10
64	Effect of pressure on the structural, electronic and mechanical properties of ultraincompressible WB.. *RSC Advances*, **2018**, 8, 35664-35671	3.7	5
63	High-Pressure Evolution of Unexpected Chemical Bonding and Promising Superconducting Properties of YB6. *Journal of Physical Chemistry C*, **2018**, 122, 27820-27828	3.8	7
62	Experimental Observation of the High Pressure Induced Substitutional Solid Solution and Phase Transformation in SbS. *Scientific Reports*, **2018**, 8, 14795	4.9	6
61	Structural metatransition of energetically tangled crystalline phases. *Physical Chemistry Chemical Physics*, **2017**, 19, 4560-4566	3.6	20

60	Anatase (101)-like Structural Model Revealed for Metastable Rutile TiO(011) Surface. *ACS Applied Materials & Interfaces*, **2017**, 9, 7891-7896	9.5	22
59	Construction of crystal structure prototype database: methods and applications. *Journal of Physics Condensed Matter*, **2017**, 29, 165901	1.8	17
58	Oxygen vacancies dependent phase transition of Y2O3 films. *Applied Surface Science*, **2017**, 410, 470-478	6.7	19
57	Extraordinary Indentation Strain Stiffening Produces Superhard Tungsten Nitrides. *Physical Review Letters*, **2017**, 119, 115503	7.4	108
56	Superconductivity in HfTe across weak to strong topological insulator transition induced via pressures. *Scientific Reports*, **2017**, 7, 44367	4.9	19
55	Pressure Driven Enhancement of Ideal Shear Strength in bc8-Carbon and Diamond. *Journal of Physical Chemistry C*, **2017**, 121, 26457-26464	3.8	6
54	Investigations on structural determination of semi-transition-metal borides. *Physical Chemistry Chemical Physics*, **2017**, 19, 31592-31598	3.6	14
53	Theoretical study of electronic and mechanical properties of Fe2B. *RSC Advances*, **2016**, 6, 73576-73580	3.7	11
52	Theoretical design of diamondlike superhard structures at high pressure. *Chinese Physics B*, **2016**, 25, 076103	1.2	5
51	Globally stable structures of LixZn (x = 1-4) compounds at high pressures. *Physical Chemistry Chemical Physics*, **2016**, 18, 4437-43	3.6	6
50	CALYPSO structure prediction method and its wide application. *Computational Materials Science*, **2016**, 112, 406-415	3.2	102
49	Low-density superhard materials: computational study of Li-inserted B-substituted closo-carboranes LiBC11 and Li2B2C10. *RSC Advances*, **2016**, 6, 52695-52699	3.7	2
48	Exploring the metallic phase of N2O under high pressure. *RSC Advances*, **2015**, 5, 65745-65749	3.7	4
47	Materials discovery via CALYPSO methodology. *Journal of Physics Condensed Matter*, **2015**, 27, 203203	1.8	63
46	Superhard-driven search of the covalent network in the B3NO system. *RSC Advances*, **2015**, 5, 35882-35887	3.7	17
45	Crystal Structures and Electronic Properties of Cesium Xenides at High Pressures. *Journal of Physical Chemistry C*, **2015**, 119, 24996-25002	3.8	12
44	Pressure-induced phase transitions and metallization in VO2. *Physical Review B*, **2015**, 91,	3.3	63
43	Pressure-induced cation-cation bonding in V2O3. *Physical Review B*, **2015**, 92,	3.3	12

42	Anomalous Stress Response of Ultrahard WB_{n} Compounds. *Physical Review Letters*, **2015**, 115, 185502	7.4	85
41	Hypervalent Iodine with Linear Chain at High Pressure. *Scientific Reports*, **2015**, 5, 14393	4.9	8
40	High pressure–low temperature phase diagram of barium: Simplicity versus complexity. *Applied Physics Letters*, **2015**, 107, 221908	3.4	7
39	Superhard BC(3) in cubic diamond structure. *Physical Review Letters*, **2015**, 114, 015502	7.4	147
38	Crystal structure and physical properties of Mo2B: First-principle calculations. *Journal of Applied Physics*, **2014**, 115, 113504	2.5	19
37	High-pressure phase transition of cesium chloride and cesium bromide. *Physical Chemistry Chemical Physics*, **2014**, 16, 17924-9	3.6	11
36	Structural and mechanical properties of platinum carbide. *Inorganic Chemistry*, **2014**, 53, 5797-802	5.1	16
35	Superconductivity of lithium-doped hydrogen under high pressure. *Acta Crystallographica Section C, Structural Chemistry*, **2014**, 70, 104-11	0.8	43
34	Exploring Hardness and the Distorted sp2 Hybridization of B–B Bonds in WB3. *Chemistry of Materials*, **2014**, 26, 5297-5302	9.6	59
33	Orthorhombic BN: A novel superhard sp3 boron nitride allotrope. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2014**, 378, 741-744	2.3	30
32	Exploring High-Pressure Structures of N2CO. *Journal of Physical Chemistry C*, **2014**, 118, 27252-27257	3.8	13
31	Unraveling Convoluted Structural Transitions in SnTe at High Pressure. *Journal of Physical Chemistry C*, **2013**, 117, 5352-5357	3.8	35
30	Orthorhombic C32: a novel superhard sp3 carbon allotrope. *Physical Chemistry Chemical Physics*, **2013**, 15, 14120-5	3.6	52
29	Enhanced Vickers hardness by quasi-3D boron network in MoB2. *RSC Advances*, **2013**, 3, 18317	3.7	42
28	Structural and electronic properties of sodium azide at high pressure: A first principles study. *Solid State Communications*, **2013**, 161, 13-18	1.6	37
27	Global structural optimization of tungsten borides. *Physical Review Letters*, **2013**, 110, 136403	7.4	216
26	Pressure-Induced Superconductivity in SnTe: A First-Principles Study. *Journal of Physical Chemistry C* , **2013**, 117, 12266-12271	3.8	24
25	First-principles structural design of superhard materials. *Journal of Chemical Physics*, **2013**, 138, 114101	3.9	151

24	Pressure-Driven Enhancement of Topological Insulating State in Tin Telluride. *Journal of Physical Chemistry C*, **2013**, 117, 8437-8442	3.8	15
23	Crystal and electronic structures of superhard B2CN : An ab initio study. *Solid State Communications* , **2012**, 152, 71-75	1.6	13
22	Direct observation of a pressure-induced precursor lattice in silicon. *Physical Review Letters*, **2012**, 109, 205503	7.4	19
21	A novel low compressible and superhard carbon nitride: body-centered tetragonal CN2. *Physical Chemistry Chemical Physics*, **2012**, 14, 13081-7	3.6	91
20	Predicted lithium-boron compounds under high pressure. *Journal of the American Chemical Society*, **2012**, 134, 18599-605	16.4	93
19	Tetragonal allotrope of group 14 elements. *Journal of the American Chemical Society*, **2012**, 134, 12362-5	16.4	146
18	B 2 CO: A potential superhard material in the B-C-O system. *Europhysics Letters*, **2011**, 95, 66006	1.6	34
17	Superhard phases of B2O: An isoelectronic compound of diamond. *Diamond and Related Materials*, **2011**, 20, 501-504	3.5	14
16	Superhard and superconductive polymorphs of diamond-like BC3. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2011**, 375, 771-774	2.3	53
15	Superhard polymorphs of diamond-like BC7. *Solid State Communications*, **2011**, 151, 716-719	1.6	34
14	Superhard and superconducting structures of BC5. *Journal of Applied Physics*, **2010**, 108, 023507	2.5	60
13	Orientationally disordered H2 in the high-pressure van der Waals compound SiH4(H2)2. *Physical Review B*, **2010**, 82,	3.3	20
12	Novel superhard polymorphs of Be3N2 predicted by first-principles. *Computational Materials Science*, **2010**, 49, S76-S79	3.2	8
11	Design of Superhard Ternary Compounds under High Pressure: SiC2N4 and Si2CN4. *Journal of Physical Chemistry C*, **2010**, 114, 8609-8613	3.8	17
10	Predicting new superhard phases. *Journal of Superhard Materials*, **2010**, 32, 192-204	0.9	40
9	Ultra-incompressible phases of tungsten dinitride predicted from first principles. *Physical Review B*, **2009**, 79,	3.3	55
8	Rhombohedral superhard structure of BC2N. *Journal of Applied Physics*, **2009**, 105, 053514	2.5	52
7	High-pressure polymorphs of Li(2)BeH(4) predicted by first-principles calculations. *Journal of Physics Condensed Matter*, **2009**, 21, 385405	1.8	3

6	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	2.8	2
5	Phase-transition mechanism of h-BN -sw-BN from first principles. *Solid State Communications*, **2009**, 149, 843-846	1.6	12
4	Superhard monoclinic polymorph of carbon. *Physical Review Letters*, **2009**, 102, 175506	7.4	434
3	Twofold coordinated ground-state and eightfold high-pressure phases of heavy transition metal nitrides MN(2) (M = Os, Ir, Ru, and Rh). *Inorganic Chemistry*, **2009**, 48, 9904-9	5.1	46
2	The effects of pressure on the electronic, transport and dynamical properties of AuX2(X = Al, Ga and In). *Journal of Physics Condensed Matter*, **2007**, 19, 425224	1.8	14
1	Ab initio prediction of superconductivity in molecular metallic hydrogen under high pressure. *Solid State Communications*, **2007**, 141, 610-614	1.6	55