

# Jian Sun

## List of Publications by Year in descending order

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124  
papers

4,538  
citations

87888

38  
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114465

63  
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127  
all docs

127  
docs citations

127  
times ranked

5024  
citing authors

#	ARTICLE	IF	CITATIONS
1	Dissecting the THz spectrum of liquid water from first principles via correlations in time and space. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 12068-12073.	7.1	374
2	Ab initio investigations of optical properties of the high-pressure phases of ZnO. Physical Review B, 2005, 71, .	3.2	363
3	Direct Band Gap Silicon Allotropes. Journal of the American Chemical Society, 2014, 136, 9826-9829.	13.7	151
4	Direct visualization of a two-dimensional topological insulator in the single-layer $T_x$ $Te_2$ . Physical Review B, 2017, 96, .	3.2	129
5	Pressure-induced superconductivity in a three-dimensional topological material ZrTe <sub>5</sub> . Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 2904-2909.	7.1	124
6	First-principles study of electronic structure and optical properties of heterodiamond BC <sub>2</sub> N. Physical Review B, 2006, 73, .	3.2	113
7	Proton-assisted growth of ultra-flat graphene films. Nature, 2020, 577, 204-208.	27.8	111
8	Conical Second Harmonic Generation in a Two-Dimensional $\Gamma_2$ Photonic Crystal: A Hexagonally Poled LiTaO <sub>3</sub> Crystal. Physical Review Letters, 2004, 93, 133904.	7.8	108
9	High-pressure polymeric phases of carbon dioxide. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 6077-6081.	7.1	104
10	A novel superhard tungsten nitride predicted by machine-learning accelerated crystal structure search. Science Bulletin, 2018, 63, 817-824.	9.0	102
11	Magnetic sensors-A review and recent technologies. Engineering Research Express, 2021, 3, 022005.	1.6	95
12	Origin of superconductivity in the Weyl semimetal $WT_2$ under pressure. Physical Review B, 2016, 94, .	3.2	91
13	Understanding THz Spectra of Aqueous Solutions: Glycine in Light and Heavy Water. Journal of the American Chemical Society, 2014, 136, 5031-5038.	13.7	88
14	Fermi Level Pinning Dependent 2D Semiconductor Devices: Challenges and Prospects. Advanced Materials, 2022, 34, e2108425.	21.0	80
15	Optical properties of heterodiamond B <sub>2</sub> CN using first-principles calculations. Applied Physics Letters, 2004, 84, 4544-4546.	3.3	78
16	Multiple superionic states in helium "water" compounds. Nature Physics, 2019, 15, 1065-1070.	16.7	69
17	Pressure-Stabilized High-Energy-Density Alkaline-Earth-Metal Pentazolate Salts. Journal of Physical Chemistry C, 2019, 123, 10205-10211.	3.1	69
18	Pressure-Induced New Topological Weyl Semimetal Phase in TaAs. Physical Review Letters, 2016, 117, 146402.	7.8	66

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19	Structural Prediction and Phase Transformation Mechanisms in Calcium at High Pressure. <i>Physical Review Letters</i> , 2009, 103, 055503.	7.8	65
20	Most likely phase of superhard $BC_2N$ calculations. <i>Physical Review B</i> , 2007, 76, .	3.2	62
21	Stable All-Nitrogen Metallic Salt at Terapascal Pressures. <i>Physical Review Letters</i> , 2013, 111, 175502.	7.8	62
22	Predictions on High-Power Trivalent Metal Pentazolate Salts. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 6166-6173.	4.6	62
23	Glycine in aqueous solution: solvation shells, interfacial water, and vibrational spectroscopy from <i>ab initio</i> molecular dynamics. <i>Journal of Chemical Physics</i> , 2010, 133, 114508.	3.0	61
24	Superconducting Single-Layer T-Graphene and Novel Synthesis Routes*. <i>Chinese Physics Letters</i> , 2019, 36, 097401.	3.3	61
25	Controlling the Bonding and Band Gaps of Solid Carbon Monoxide with Pressure. <i>Physical Review Letters</i> , 2011, 106, 145502.	7.8	60
26	Structural transformations in carbon under extreme pressure: Beyond diamond. <i>Journal of Chemical Physics</i> , 2009, 130, 194512.	3.0	56
27	Solvothermal Synthesis of Lateral Heterojunction $Sb_2Te_3/Bi_2Te_3$ Nanoplates. <i>Nano Letters</i> , 2015, 15, 5905-5911.	9.1	56
28	Comment on "New Metallic Carbon Crystal". <i>Physical Review Letters</i> , 2009, 102, 229601.	7.8	55
29	Persistence and Eventual Demise of Oxygen Molecules at Terapascal Pressures. <i>Physical Review Letters</i> , 2012, 108, 045503.	7.8	55
30	High efficiency single- and dual-wavelength $Nd:GdVO_4$ lasers pumped by a fiber-coupled diode. <i>Applied Physics B: Lasers and Optics</i> , 2004, 79, 301-304.	2.2	54
31	Pressure-induced metallization and superconducting phase in $ReS_2$ . <i>Npj Quantum Materials</i> , 2017, 2, .	5.2	53
32	Tungsten Hexanitride with Single-Bonded Armchairlike Hexazine Structure at High Pressure. <i>Physical Review Letters</i> , 2021, 126, 065702.	7.8	52
33	Concurrence of superconductivity and structure transition in Weyl semimetal $TaP$ under pressure. <i>Npj Quantum Materials</i> , 2017, 2, .	5.2	47
34	Solvation shell resolved THz spectra of simple aqua ions " distinct distance- and frequency-dependent contributions of solvation shells. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 8323-8329.	2.8	45
35	Tunable electronic structure of two-dimensional transition metal chalcogenides for optoelectronic applications. <i>Nanophotonics</i> , 2020, 9, 1675-1694.	6.0	44
36	Bond ionicities and hardness of $B_13C_2$ -like structured $ByX$ crystals ( $X=C,N,O,P,As$ ). <i>Physical Review B</i> , 2006, 73, .	3.2	42

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37	Chalcopyrite polymorph for superhard BC2N. Applied Physics Letters, 2006, 89, 151911.	3.3	41
38	Understanding the Origins of Dipolar Couplings and Correlated Motion in the Vibrational Spectrum of Water. Journal of Physical Chemistry Letters, 2012, 3, 2135-2140.	4.6	41
39	Strain-induced quantum topological phase transitions in Na3Bi. Physical Review B, 2017, 96, .	3.2	37
40	Theoretical hardness of the cubic BC2N. Diamond and Related Materials, 2007, 16, 526-530.	3.9	36
41	Topological Dirac line nodes and superconductivity coexist in SnSe at high pressure. Physical Review B, 2017, 96, .	3.2	35
42	Evidence for a Dirac nodal-line semimetal in SrAs3. Science Bulletin, 2018, 63, 535-541.	9.0	34
43	Self-Terminated Surface Monolayer Oxidation Induced Robust Degenerate Doping in MoTe <sub>2</sub> for Low Contact Resistance. ACS Applied Materials & Interfaces, 2020, 12, 26586-26592.	8.0	34
44	Structures and superconducting properties of the high-pressure IV and V phases of calcium from first principles. Physical Review B, 2008, 78, .	3.2	33
45	Coexistence of plastic and partially diffusive phases in a helium-methane compound. National Science Review, 2020, 7, 1540-1547.	9.5	33
46	A tetragonal phase of superhard BC2N. Journal of Applied Physics, 2009, 105, .	2.5	32
47	Charge-Ordered Ferroelectric Transition in Ultrathin Na <sub>0.5</sub> Bi <sub>4.5</sub> Ti <sub>4</sub> O <sub>15</sub> Flakes Probed via a Dual-Gated Full van der Waals Transistor. Advanced Materials, 2020, 32, e2004813.	21.0	28
48	Plastic and Superionic Helium Ammonia Compounds under High Pressure and High Temperature. Physical Review X, 2020, 10, .	8.9	28
49	Epitaxial Growth of Single-Phase 1T' WSe <sub>2</sub> Monolayer with Assistance of Enhanced Interface Interaction. Advanced Materials, 2021, 33, e2004930.	21.0	28
50	High performance WSe <sub>2</sub> p-MOSFET with intrinsic n-channel based on back-to-back pn junctions. Applied Physics Letters, 2021, 118, .	3.3	26
51	Enhancing crystal structure prediction by decomposition and evolution schemes based on graph theory. Fundamental Research, 2021, 1, 466-471.	3.3	23
52	Ground state structure of high-energy-density polymeric carbon monoxide. Physical Review B, 2017, 95, .	3.2	22
53	Predicting three-dimensional icosahedron-based boron $B_{60}$ . Physical Review B, 2019, 99, .	3.2	21
54	Gate Tunable Hole Charge Qubit Formed in a Ge/Si Nanowire Double Quantum Dot Coupled to Microwave Photons. Nano Letters, 2019, 19, 1052-1060.	9.1	20

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55	Charge Density Depinning in Defective MoTe <sub>2</sub> Transistor by Oxygen Intercalation. <i>Advanced Functional Materials</i> , 2020, 30, 2004880.	14.9	20
56	Mixed Coordination Silica at Megabar Pressure. <i>Physical Review Letters</i> , 2021, 126, 035701.	7.8	20
57	Prediction of pressure-induced stabilization of noble-gas-atom compounds with alkali oxides and alkali sulfides. <i>Physical Review Materials</i> , 2019, 3, .	2.4	20
58	Helical Hole State in Multiple Conduction Modes in Ge/Si Core/Shell Nanowire. <i>Nano Letters</i> , 2018, 18, 6144-6149.	9.1	19
59	Growth and Thermo-driven Crystalline Phase Transition of Metastable Monolayer 1Tâ€²-WSe <sub>2</sub> Thin Film. <i>Scientific Reports</i> , 2019, 9, 2685.	3.3	19
60	Experimental evidence of crystal symmetry protection for the topological nodal line semimetal state in ZrSiS. <i>Physical Review B</i> , 2019, 100, .	3.2	19
61	High-energy-density pentazolates: CaN <sub>10</sub> and BaN <sub>10</sub> . <i>Science China: Physics, Mechanics and Astronomy</i> , 2021, 64, 1.	5.1	19
62	Superionic Silica-Water and Silica-Hydrogen Compounds in the Deep Interiors of Uranus and Neptune. <i>Physical Review Letters</i> , 2022, 128, 035702.	7.8	19
63	Evidence for magnon-phonon coupling in the topological magnet $\langle \text{mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:msub} \rangle \langle \text{mml:mi} \rangle \text{Cu} \langle \text{mml:mi} \rangle \langle \text{mml:mns} \rangle \langle \text{mml:mn} \rangle \langle \text{mml:m} \rangle \langle \text{mml:msup} \rangle \langle \text{mml:mi} \rangle \text{Cu}$ . <i>Physical Review B</i> , 2020, 101, .	3.2	18
64	Reconfigurable Quasi-Nonvolatile Memory/Subthermionic FET Functions in Ferroelectricâ€²D Semiconductor vdW Architectures. <i>Advanced Materials</i> , 2022, 34, e2200032.	21.0	18
65	Infrared and Raman spectra of $\text{BC}_2\text{N}$ from first principles calculations. <i>Physical Review B</i> , 2006, 74, .	3.2	17
66	Unveiling the charge density wave inhomogeneity and pseudogap state in 1 T -TiSe <sub>2</sub> . <i>Science Bulletin</i> , 2018, 63, 426-432.	9.0	17
67	Novel electronic and phonon-related properties of the newly discovered silicide superconductor Li <sub>2</sub> IrSi <sub>3</sub> . <i>Europhysics Letters</i> , 2015, 110, 17003.	2.0	16
68	High-pressure phases of Weyl semimetals NbP, NbAs, TaP, and TaAs. <i>Science China: Physics, Mechanics and Astronomy</i> , 2018, 61, 1.	5.1	16
69	Pressure-induced structural and electronic transitions in bismuth iodide. <i>Physical Review B</i> , 2018, 98, .	3.2	15
70	Electrostatic force driven helium insertion into ammonia and water crystals under pressure. <i>Communications Chemistry</i> , 2019, 2, .	4.5	15
71	Ambipolar MoS <sub>2</sub> Field-Effect Transistor by Spatially Controlled Chemical Doping. <i>Physica Status Solidi - Rapid Research Letters</i> , 2019, 13, 1900208.	2.4	15
72	Formation of copper boride on Cu(111). <i>Fundamental Research</i> , 2021, 1, 482-487.	3.3	15

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73	Tunable large-area phase reversion in chemical vapor deposited few-layer MoTe <sub>2</sub> films. Journal of Materials Chemistry C, 2019, 7, 10598-10604.	5.5	14
74	Improve the performance of machine-learning potentials by optimizing descriptors. Journal of Chemical Physics, 2019, 150, 244110.	3.0	14
75	High-pressure structures and vibrational spectra of barium fluoride: Results obtained under nearly hydrostatic conditions. Physical Review B, 2009, 79, .	3.2	13
76	Superhard and superconducting B6C. Materials Today Physics, 2017, 3, 76-84.	6.0	13
77	Ferromagnetic MnSn Monolayer Epitaxially Grown on Silicon Substrate. Chinese Physics Letters, 2020, 37, 077502.	3.3	13
78	Pressure-induced anomalous enhancement of insulating state and isosymmetric structural transition in quasi-one-dimensional $TiS_3$ . Physical Review B, 2017, 96, .	3.2	12
79	Nonsymmorphic symmetry protected node-line semimetal in the trigonal YH3. Scientific Reports, 2018, 8, 1467.	3.3	12
80	Prediction of quasi-one-dimensional superconductivity in metastable two-dimensional boron. Physical Review B, 2020, 101, .	3.2	12
81	Electronically Driven 1D Cooperative Diffusion in a Simple Cubic Crystal. Physical Review X, 2021, 11, .	8.9	12
82	Novel structural phases and superconductivity of iridium telluride under high pressures. Scientific Reports, 2014, 4, 6433.	3.3	11
83	Silicon clathrates for photovoltaics predicted by a two-step crystal structure search. Applied Physics Letters, 2017, 111, 173904.	3.3	11
84	Composite topological nodal lines penetrating the Brillouin zone in orthorhombic AgF2. Npj Computational Materials, 2019, 5, .	8.7	11
85	Van Hove singularity arising from Mexican-hat-shaped inverted bands in the topological insulator Sn-doped $Bi_{1-x}Sb_x$ . Physical Review B, 2020, 101, .	3.2	11
86	Unusual phonon density of states and response to the superconducting transition in the In-doped topological crystalline insulator $Pb_{1-x}Sn_x$ . Physical Review B, 2018, 97, .	3.2	10
87	Quantum Dot Formation in Controllably Doped Graphene Nanoribbon. ACS Nano, 2019, 13, 7502-7507.	14.6	10
88	Directly Probing Effective-Mass Anisotropy of Two-Dimensional $ReSe_2$ in Schottky Tunnel Transistors. Physical Review Applied, 2020, 13, .	3.8	10
89	High-energy-density metal nitrides with armchair chains. Matter and Radiation at Extremes, 2022, 7, .	3.9	10
90	Ground states of Au <sub>2</sub> Pb and pressure-enhanced superconductivity. Physical Review B, 2019, 100, .	3.2	9

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91	Pressure-induced multiband superconductivity in pyrite $\text{PtB}_2$ with perfect electron-hole compensation. <i>Physical Review Materials</i> , 2018, 2, .	2.4	9
92	Pressure Induced Enhancement of Superconductivity in $\text{LaRu}_2\text{P}_2$ . <i>Scientific Reports</i> , 2016, 6, 24479.	3.3	8
93	High-temperature superconducting phase of HBr under pressure predicted by first-principles calculations. <i>Physical Review B</i> , 2017, 96, .	3.2	8
94	Determining dimensionalities and multiplicities of crystal nets. <i>Npj Computational Materials</i> , 2020, 6, .	8.7	8
95	Asymmetric Fermi velocity induced chiral magnetotransport anisotropy in the type-II Dirac semi-metal $\text{PtSe}_2$ . <i>Communications Physics</i> , 2020, 3, .	5.3	8
96	Modulated Anisotropic Growth of 2D $\text{SnSe}$ Based on the Difference in $a$ / $b$ / $c$ -Axis Edge Atomic Structures. <i>Chemistry of Materials</i> , 2021, 33, 4231-4239.	6.7	8
97	High Energy Density Polymeric Nitrogen Nanotubes inside Carbon Nanotubes. <i>Chinese Physics Letters</i> , 2022, 39, 036101.	3.3	8
98	Phonon density of states of single-crystal $\text{SrF}_2$ across the collapsed phase transition at high pressure. <i>Physical Review B</i> , 2016, 94, .	3.2	7
99	Anharmonic effect driven topological phase transition in $\text{PbO}_2$ predicted by first-principles calculations. <i>Physical Review B</i> , 2018, 98, .	3.2	7
100	The influence of tensile strain on water adsorbed on Fe (100) surface: Surface chemistry aspect of stress corrosion cracking. <i>Applied Surface Science</i> , 2019, 481, 192-199.	6.1	7
101	Ferromagnetic Semiconducting $\text{V}_3$ Single-Chain Nanowire. <i>Journal of Physical Chemistry C</i> , 2020, 124, 2096-2103.	3.1	7
102	Topological insulators in the $\text{NaCaBi}$ family with large spin-orbit coupling gaps. <i>Physical Review Research</i> , 2021, 3, .	3.6	7
103	Controlling Carrier Transport in Vertical $\text{MoTe}_2$ / $\text{MoS}_2$ van der Waals Heterostructures. <i>ACS Applied Materials &amp; Interfaces</i> , 2021, 13, 54294-54300.	8.0	7
104	Nanocrystalline tin oxide: Possible origin of its weak ferromagnetism deduced from nuclear magnetic resonance and X-ray photoelectron spectroscopies. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2016, 380, 3138-3143.	2.1	6
105	Electron-phonon coupling and superconductivity in the doped topological crystalline insulator $(\text{Pb}_{0.5}\text{Sn}_{0.5})_2\text{In}_x\text{Te}$ . <i>Physical Review B</i> , 2020, 102, .	3.2	5
106	Pressure engineering of the Dirac fermions in quasi-one-dimensional $\text{Tl}_2\text{Mo}_6\text{Se}_6$ . <i>Journal of Physics Condensed Matter</i> , 2020, 32, 215402.	1.8	5
107	Structural evolution behavior of manganese monophosphide under high pressure: experimental and theoretical study. <i>Journal of Physics Condensed Matter</i> , 2017, 29, 254002.	1.8	4
108	Electrically tunable localized states in sub-band of bilayer graphene nanoribbon. <i>Applied Physics Letters</i> , 2018, 113, .	3.3	4

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109	Icosahedral silicon boride: A potential hybrid photovoltaic-thermoelectric for energy harvesting. <i>Physical Review Materials</i> , 2021, 5, .	2.4	4
110	Temperature-induced electricle transition in dense lithium. <i>Physical Review B</i> , 2022, 105, .	3.2	4
111	Quantum oscillations on the surface of InAs epilayer. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2019, 114, 113604.	2.7	3
112	Robust double Weyl semimetal phase in a nonmagnetic hexagonal lattice system. <i>Physical Review B</i> , 2019, 99, .	3.2	3
113	Spin filtering in germanium/silicon core/shell nanowires with pseudo-helical gap. <i>Applied Physics Letters</i> , 2020, 117, .	3.3	3
114	Pressure-induced structural and electronic transitions in InTe. <i>Physical Review B</i> , 2021, 104, .	3.2	3
115	Partially Diffusive Helium-Silica Compound under High Pressure. <i>Chinese Physics Letters</i> , 0, , .	3.3	3
116	Double quantum dot-like transport in controllably doped graphene nanoribbon. <i>Applied Physics Letters</i> , 2021, 118, .	3.3	2
117	Comprehensive Modulation of Conductance Anisotropy in Low-Symmetry $\langle \text{mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" overflow="scroll">\langle \text{mml:mrow}>\langle \text{mml:mi}>R\langle \text{mml:mi}>\langle \text{mml:mi mathvariant="normal">S}\langle \text{mml:mi}>\langle \text{mml:mrow}>\langle \text{mml:mn}>2\langle \text{mml:mn}>\langle \text{mml:mrow}>\langle \text{mml:math}>$ Transistors. <i>Physical Review Applied</i> , 2022, 17, .	3.8	2
118	Isotropic all-electric spin analyzer based on a quantum ring with spin-orbit couplings. <i>Applied Physics Letters</i> , 2021, 118, .	3.3	1
119	Filamentary superconductivity in wrinkled PtSe <sub>2</sub> . <i>Journal Physics D: Applied Physics</i> , 2021, 54, 215302.	2.8	1
120	Negative linear compressibility and unusual dynamic behavior of NaB <sub>3</sub> . <i>Physical Review Materials</i> , 2021, 5, .	2.4	1
121	Current-Induced Complementary Doping to Graphene from Hydrogen Silsesquioxane Passivation Layer. <i>Physica Status Solidi - Rapid Research Letters</i> , 2021, 15, 2100151.	2.4	1
122	Yao <i>et al.</i> Reply. <i>Physical Review Letters</i> , 2010, 104, .	7.8	0
123	Route to a novel tetragonal carbon allotrope via T-carbon. <i>Diamond and Related Materials</i> , 2022, , 108895.	3.9	0
124	Pressure-induced phase transitions in the ZrXY (X= Si, Ge, Sn; Y= S, Se, Te) family compounds. <i>Chinese Physics B</i> , 0, , .	1.4	0