

# Jian-Tao Wang

## List of Publications by Year in descending order

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82  
papers

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citations

304743

22  
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254184

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docs citations

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times ranked

1765  
citing authors

#	ARTICLE	IF	CITATIONS
1	Low-Temperature Phase Transformation from Graphite to $\sqrt{3} \times \sqrt{3}$ Orthorhombic Carbon. Physical Review Letters, 2011, 106, 075501.	7.8	259
2	Body-Centered Orthorhombic $\sqrt{2} \times \sqrt{2} \times \sqrt{2}$ A Novel Topological Node-Line Semimetal. Physical Review Letters, 2016, 116, 195501.	7.8	170
3	Prediction of a new two-dimensional metallic carbon allotrope. Physical Chemistry Chemical Physics, 2013, 15, 2024-2030.	2.8	124
4	Topological Nodal-Net Semimetal in a Graphene Network Structure. Physical Review Letters, 2018, 120, 026402.	7.8	93
5	Orthorhombic carbon allotrope of compressed graphite: <i>Ab initio</i> calculations. Physical Review B, 2012, 85, .	3.2	80
6	A New Carbon Allotrope with Six-Fold Helical Chains in all-sp <sup>2</sup> Bonding Networks. Scientific Reports, 2014, 4, 4339.	3.3	77
7	H18 Carbon: A New Metallic Phase with sp <sup>2</sup> -sp <sup>3</sup> Hybridized Bonding Network. Scientific Reports, 2016, 6, 21879.	3.3	57
8	New Carbon Allotropes with Helical Chains of Complementary Chirality Connected by Ethene-type $\pi$ -Conjugation. Scientific Reports, 2013, 3, 3077.	3.3	52
9	K6 carbon: A metallic carbon allotrope in sp <sup>3</sup> bonding networks. Journal of Chemical Physics, 2014, 140, 054514.	3.0	52
10	Mechanism for direct graphite-to-diamond phase transition. Scientific Reports, 2014, 4, 5930.	3.3	52
11	Computational prediction of body-centered cubic carbon in an all- $\sqrt{2} \times \sqrt{2} \times \sqrt{2}$ ring configuration. Physical Review B, 2015, 91, .	3.2	49
12	Orthorhombic carbon oC24: A novel topological nodal line semimetal. Carbon, 2018, 133, 39-43.	10.3	48
13	Kinetic Origin of Divergent Decompression Pathways in Silicon and Germanium. Physical Review Letters, 2013, 110, 165503.	7.8	44
14	Phase conversion from graphite toward a simple monoclinic <i>sp</i> <sup>3</sup> -carbon allotrope. Journal of Chemical Physics, 2012, 137, 024502.	3.0	38
15	Mechanism for direct conversion of graphite to diamond. Physical Review B, 2011, 84, .	3.2	34
16	New carbon allotropes in sp + sp <sup>3</sup> bonding networks consisting of C <sub>8</sub> cubes. Physical Chemistry Chemical Physics, 2018, 20, 7962-7967.	2.8	33
17	Phase stability of carbon clathrates at high pressure. Journal of Applied Physics, 2010, 107, .	2.5	31
18	Magic Monatomic Linear Chains for Mn Nanowire Self-Assembly on Si(001). Physical Review Letters, 2010, 105, 116102.	7.8	30

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19	First-principles study of point defects in solar cell semiconductor CuInS <sub>2</sub> . Journal of Applied Physics, 2012, 112, .	2.5	30
20	New cubic carbon phase via graphitic sheet rumpling. Physical Review B, 2012, 85, .	3.2	30
21	Three-Dimensional Carbon Allotropes Comprising Phenyl Rings and Acetylenic Chains in sp+sp <sup>2</sup> Hybrid Networks. Scientific Reports, 2016, 6, 24665.	3.3	29
22	Topological nodal line semimetal in an orthorhombic graphene network structure. Physical Review B, 2018, 97, .	3.2	29
23	Monoclinic $\text{EuSn}_2$ : A Novel High-Pressure Network Structure. Physical Review Letters, 2021, 126, 155701.	7.8	21
24	Large Enhancement of Magnetocaloric and Barocaloric Effects by Hydrostatic Pressure in La(Fe <sub>0.92</sub> Co <sub>0.08</sub> ) <sub>11.9</sub> Si <sub>1.1</sub> with a NaZn <sub>13</sub> -Type Structure. Chemistry of Materials, 2020, 32, 1807-1818.	6.7	23
25	Computational discovery of a new rhombohedral diamond phase. Physical Review B, 2018, 98, .	3.2	22
26	Dynamic Ad-Dimer Twisting Assisted Nanowire Self-Assembly on Si(001). Physical Review Letters, 2005, 94, 226103.	7.8	21
27	Body centered cubic carbon BC14: An all- <i>s</i> -bonded full-fledged pentadiamond. Physical Review B, 2020, 102, .	3.2	21
28	Highly stable and symmetric boron caged B@Co <sub>12</sub> @B <sub>80</sub> core-shell cluster. Applied Physics Letters, 2009, 94, 133102.	3.3	19
29	Giant Magnetic Quantum Oscillations in the Thermal Conductivity of TaAs: Indications of Chiral Zero Sound. Physical Review X, 2019, 9, .	8.9	19
30	A superhard orthorhombic carbon with all six-membered-ring in sp <sup>3</sup> bonding networks. Physics Letters, Section A: General, Atomic and Solid State Physics, 2019, 383, 2809-2812.	2.1	19
31	Cone-spiral magnetic ordering dominated lattice distortion and giant negative thermal expansion in Fe-doped MnNiGe compounds. Materials Horizons, 2020, 7, 804-810.	12.2	19
32	Vacancy-assisted diffusion mechanism of group-III elements in ZnO: An ab initio study. Journal of Applied Physics, 2009, 105, 073504.	2.5	18
33	Hydrogenated <i>K</i> <sub>4</sub> carbon: A new stable cubic gauche structure of carbon hydride. Journal of Chemical Physics, 2013, 138, 024702.	3.0	18
34	<i>Ab initio</i> prediction of superdense tetragonal and monoclinic polymorphs of carbon. Physical Review B, 2016, 94, .	3.2	18
35	Topological semimetal in an <i>s</i> - <i>p</i> <sup>2</sup> hybridized carbon network with nodal rings. Physical Review B, 2020, 101, .	3.2	18
36	Stability of Sb line structures on Si(001). Physical Review B, 2003, 67, .	3.2	17

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37	Three-Dimensional Crystalline Modification of Graphene in all-sp <sup>2</sup> Hexagonal Lattices with or without Topological Nodal Lines. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 2515-2521.	4.6	16
38	Dimensional crossover tuned by pressure in layered magnetic NiPS <sub>3</sub> . <i>Science China: Physics, Mechanics and Astronomy</i> , 2021, 64, 1.	5.1	16
39	Structural and electronic properties of linear and angular polycyclic aromatic hydrocarbons. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2014, 378, 1379-1382.	2.1	13
40	Ab Initio Study of Water Adsorption and Reactivity on the (211) Surface of Anatase TiO <sub>2</sub> . <i>Physical Review Applied</i> , 2016, 5, .	3.8	12
41	Hybrid nodal chain in an orthorhombic graphene network. <i>Physical Review B</i> , 2021, 103, .	3.2	12
42	First-principles studies on the structural and magnetic properties of (Cr, Mn, Fe)/Ag monatomic multilayers. <i>Journal of Physics Condensed Matter</i> , 1998, 10, 9655-9662.	1.8	10
43	Two-Stage Rotation Mechanism for Group-V Precursor Dissociation on Si(001). <i>Physical Review Letters</i> , 2006, 97, 046103.	7.8	10
44	Ab initio study of the anharmonic lattice dynamics of iron at the $\bar{1}3\bar{a}^{\prime}\bar{1}$ phase transition. <i>Physical Review B</i> , 2015, 92, .	3.2	10
45	Phase stability and transition of BaSi <sub>2</sub> disilicides and digermanides. <i>Physical Review B</i> , 2015, 91, .	3.1	10
46	Novel electronic properties of monoclinic MP <sub>4</sub> (M = Cr, Mo, W) compounds with or without topological nodal line. <i>Scientific Reports</i> , 2020, 10, 11502.	3.3	10
47	Crystalline structures of polymeric hydrocarbon with 3,4-fold helical chains. <i>Scientific Reports</i> , 2015, 5, 7723.	3.3	9
48	A new carbon allotrope with orthorhombic symmetry formed via graphitic sheet buckling. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 22762-22767.	2.8	9
49	Topological nodal line semimetals in graphene network structures. <i>Advances in Physics: X</i> , 2019, 4, 1625724.	4.1	9
50	Molecular orbital analysis of frontier orbitals for molecular electronics: a case study of unimolecular rectifier and photovoltaic cell. <i>Science and Technology of Advanced Materials</i> , 2003, 4, 377-382.	6.1	8
51	Magnetic and electronic properties of Cr, Mn, and Fe adatoms on Si(001): A first-principles study. <i>Solid State Communications</i> , 2012, 152, 127-131.	1.9	8
52	Three-dimensional polymeric structures of single-wall carbon nanotubes. <i>Journal of Chemical Physics</i> , 2014, 140, 204709.	3.0	8
53	Pressure-driven electronic and structural phase transition in intrinsic magnetic topological insulator MnSb. <i>Physical Review B</i> , 2021, 104, .	3.2	8
54	Adsorption, diffusion, and site exchange for Ge ad-dimers on Sb-covered Si(001) from first-principles total-energy calculations. <i>Physical Review B</i> , 2006, 74, .	3.2	7

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55	Size-selective self-assembly of magnetic Mn nanoclusters on Si(111). Journal of Chemical Physics, 2013, 138, 164705. Topological nodal surface semimetal states in $\text{Sr}_5\text{Sb}_2\text{Te}_9$ compounds	3.0	7
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73	Self-assembly of glycine on Cu(001): the effect of temperature and polarity. RSC Advances, 2017, 7, 4116-4123.	3.6	3
74	New carbon allotropes derived from nanotubes via a three-fold distortion mechanism. Physical Chemistry Chemical Physics, 2020, 22, 12489-12495.	2.8	2
75	Structural and electronic properties of BaSi <sub>2</sub> (100) thin film on Si(111) substrate. Journal of Materials Science, 2020, 55, 9483-9492.	3.7	2
76	First-Principles Study of the Electronic Properties of $\gamma$ - $\gamma'$ Interface in Ni Based Superalloys. Materials Transactions, 2005, 46, 1122-1126.	1.2	1
77	Structural stability and electronic properties of Sr induced (5 $\times$ 4) reconstruction on Si(111) surface. Physics Letters, Section A: General, Atomic and Solid State Physics, 2020, 384, 126540.	2.1	1
78	La induced Si <sub>3</sub> trimer bilayer on the Si(111) surface. Physical Chemistry Chemical Physics, 2021, 23, 11466-11471.	2.8	1
79	La induced Si <sub>3</sub> trimer monolayer on Si(111) surface: An ab initio study. New Journal of Physics, 0, , .	2.9	1
80	Dynamic formation process of Bi line structure on Si(100) surface. Computational Materials Science, 2006, 36, 135-138.	3.0	0
81	Structural and electronic properties of XP <sub>4</sub> (X = Ru, Os) compounds. Solid State Communications, 2021, 326, 114173.	1.9	0
82	Structural stability and electronic properties of Er nanowire on Si(001). Physica E: Low-Dimensional Systems and Nanostructures, 2022, , 115233.	2.7	0