

Jian-Tao Wang

List of Publications by Year in descending order

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#	ARTICLE	IF	CITATIONS
1	Structural, magnetic, and electronic properties of EuSi_2 thin films on the Si(111) surface. Physical Chemistry Chemical Physics, 2022, 24, 6782-6787.	2.8	6
2	Topological nodal line semimetal in an all-sp ² monoclinic carbon. New Journal of Physics, 2022, 24, 043007.	2.9	4
3	Structural stability and electronic properties of Er nanowire on Si(001). Physica E: Low-Dimensional Systems and Nanostructures, 2022, 115233.	2.7	0
4	Topological nodal surface semimetal states in Sr_5 compounds		

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19	New carbon allotropes derived from nanotubes via a three-fold distortion mechanism. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 12489-12495.	2.8	2
20	Structural and electronic properties of BaSi ₂ (100) thin film on Si(111) substrate. <i>Journal of Materials Science</i> , 2020, 55, 9483-9492.	3.7	2
21	Structural stability and electronic properties of Sr induced (5Å ⁻⁴) reconstruction on Si(111) surface. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2020, 384, 126540.	2.1	1
22	Large Enhancement of Magnetocaloric and Barocaloric Effects by Hydrostatic Pressure in La(Fe _{0.92} Co _{0.08}) _{11.9} Si _{1.1} with a NaZn ₁₃ -Type Structure. <i>Chemistry of Materials</i> , 2020, 32, 1807-1818.	6.7	23
23	Mn-Doped Sr/Si(111)-(3 Å ⁻²) HCC Surfaces: Antiferromagnetic Semiconductors for Spintronic Applications. <i>ACS Applied Materials & Interfaces</i> , 2020, 12, 9918-9924.	8.0	5
24	Topological nodal line semimetals in graphene network structures. <i>Advances in Physics: X</i> , 2019, 4, 1625724.	4.1	9
25	Giant Magnetic Quantum Oscillations in the Thermal Conductivity of TaAs: Indications of Chiral Zero Sound. <i>Physical Review X</i> , 2019, 9, .	8.9	19
26	A superhard orthorhombic carbon with all six-membered-ring in sp ³ bonding networks. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2019, 383, 2809-2812.	2.1	19
27	Three-Dimensional Crystalline Modification of Graphene in all-sp ² Hexagonal Lattices with or without Topological Nodal Lines. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 2515-2521.	4.6	16
28	Orthorhombic carbon oC ₂₄ : A novel topological nodal line semimetal. <i>Carbon</i> , 2018, 133, 39-43.	10.3	48
29	New carbon allotropes in sp + sp ³ bonding networks consisting of C ₈ cubes. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 7962-7967.	2.8	33
30	Topological Nodal-Net Semimetal in a Graphene Network Structure. <i>Physical Review Letters</i> , 2018, 120, 026402.	7.8	93
31	Structural stability and electronic properties of alkaline-earth metal induced Si(111)-(3 Å ⁻²) surfaces. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 25235-25239.	2.8	6
32	Computational discovery of a new rhombohedral diamond phase. <i>Physical Review B</i> , 2018, 98, .	3.2	22
33	Topological nodal line semimetal in an orthorhombic graphene network structure. <i>Physical Review B</i> , 2018, 97, .	3.2	29
34	A new carbon allotrope with orthorhombic symmetry formed <i>via</i> graphitic sheet buckling. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 22762-22767.	2.8	9
35	Self-assembly of glycine on Cu(001): the effect of temperature and polarity. <i>RSC Advances</i> , 2017, 7, 4116-4123.	3.6	3
36	Phonon-mediated high-T _c superconductivity in hole-doped diamond-like crystalline hydrocarbon. <i>Scientific Reports</i> , 2017, 7, 1464.	3.3	6

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37	Computational prediction of a simple cubic carbon allotrope consisting of C12 clusters. Journal of Chemical Physics, 2017, 147, 064512.	3.0	6
38	H18 Carbon: A New Metallic Phase with sp ² -sp ³ Hybridized Bonding Network. Scientific Reports, 2016, 6, 21879.	3.3	57
39	Three-Dimensional Carbon Allotropes Comprising Phenyl Rings and Acetylenic Chains in sp+sp ² Hybrid Networks. Scientific Reports, 2016, 6, 24665.	3.3	29
40	Body-Centered Orthorhombic C_{16} A Novel Topological Node-Line Semimetal. Physical Review Letters, 2016, 116, 195501.	7.8	170
41	<i>Ab Initio</i> Study of Water Adsorption and Reactivity on the (211) Surface of Anatase TiO ₂ . Physical Review Applied, 2016, 5, .	3.8	12
42	<i>Ab initio</i> prediction of superdense tetragonal and monoclinic polymorphs of carbon. Physical Review B, 2016, 94, .	3.2	18
43	<i>Ab initio</i> study of the anharmonic lattice dynamics of iron at the β phase transition. Physical Review B, 2015, 92, .	3.2	10
44	Computational prediction of body-centered cubic carbon in an all-sps ² ring configuration. Physical Review B, 2015, 91, .	3.2	10
45	Crystalline structures of polymeric hydrocarbon with 3,4-fold helical chains. Scientific Reports, 2015, 5, 7723.	3.3	9
46	Phase stability and transition of BaSi ₂ disilicides and digermanides. Physical Review B, 2015, 91, .	3.1	10
47	Three-dimensional polymeric structures of single-wall carbon nanotubes. Journal of Chemical Physics, 2014, 140, 204709.	3.0	8
48	Structural and electronic properties of linear and angular polycyclic aromatic hydrocarbons. Physics Letters, Section A: General, Atomic and Solid State Physics, 2014, 378, 1379-1382.	2.1	13
49	K6 carbon: A metallic carbon allotrope in sp ³ bonding networks. Journal of Chemical Physics, 2014, 140, 054514.	3.0	52
50	A New Carbon Allotrope with Six-Fold Helical Chains in all-sp ² Bonding Networks. Scientific Reports, 2014, 4, 4339.	3.3	77
51	Mechanism for direct graphite-to-diamond phase transition. Scientific Reports, 2014, 4, 5930.	3.3	52
52	Prediction of a new two-dimensional metallic carbon allotrope. Physical Chemistry Chemical Physics, 2013, 15, 2024-2030.	2.8	124
53	New Carbon Allotropes with Helical Chains of Complementary Chirality Connected by Ethene-type π -Conjugation. Scientific Reports, 2013, 3, 3077.	3.3	52
54	Size-selective self-assembly of magnetic Mn nanoclusters on Si(111). Journal of Chemical Physics, 2013, 138, 164705.	3.0	7

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55	Hydrogenated K_4 carbon: A new stable cubic gauche structure of carbon hydride. Journal of Chemical Physics, 2013, 138, 024702.	3.0	18
56	Kinetic Origin of Divergent Decompression Pathways in Silicon and Germanium. Physical Review Letters, 2013, 110, 165503.	7.8	44
57	First-principles study of point defects in solar cell semiconductor CuInS ₂ . Journal of Applied Physics, 2012, 112, .	2.5	30
58	Phase conversion from graphite toward a simple monoclinic sp^3 -carbon allotrope. Journal of Chemical Physics, 2012, 137, 024502.	3.0	38
59	Orthorhombic carbon allotrope of compressed graphite: <i>Ab initio</i> calculations. Physical Review B, 2012, 85, .	3.2	80
60	New cubic carbon phase via graphitic sheet rumpling. Physical Review B, 2012, 85, .	3.2	30
61	Magnetic and electronic properties of Cr, Mn, and Fe adatoms on Si(001): A first-principles study. Solid State Communications, 2012, 152, 127-131.	1.9	8
62	Mechanism for direct conversion of graphite to diamond. Physical Review B, 2011, 84, .	3.2	34
63	Low-Temperature Phase Transformation from Graphite to sp^3 Carbon. Physical Review Letters, 2011, 106, 075501.	7.8	259
64	Adsorption of Au and Pt dimers on Ge(001) and Si(001): A first-principles study. Solid State Communications, 2011, 151, 655-658.	1.9	3
65	Atomistic nucleation and growth mechanism for single-wall carbon nanotubes on catalytic nanoparticle surfaces. Nanotechnology, 2010, 21, 115602.	2.6	6
66	Phase stability of carbon clathrates at high pressure. Journal of Applied Physics, 2010, 107, .	2.5	31
67	Magic Monatomic Linear Chains for Mn Nanowire Self-Assembly on Si(001). Physical Review Letters, 2010, 105, 116102.	7.8	30
68	Highly stable and symmetric boron caged B@Co ₁₂ @B ₈₀ core-shell cluster. Applied Physics Letters, 2009, 94, 133102.	3.3	19
69	Vacancy-assisted diffusion mechanism of group-III elements in ZnO: An <i>ab initio</i> study. Journal of Applied Physics, 2009, 105, 073504.	2.5	18
70	Formation of Ga dimer linear chains on Si(001): a first-principles study. Journal of Physics Condensed Matter, 2008, 20, 445002.	1.8	3
71	Effect of strain on the energetics and kinetics of dissociation of Sb_4 Ge(001). Physical Review B, 2008, 78, .	3.2	3
72	Dimer-breaking-assisted exchange mechanism in surfactant-mediated epitaxial growth of Ge on Si(001): <i>Ab initio</i> total energy calculations. Physical Review B, 2007, 76, .	3.2	3

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73	Two-Stage Rotation Mechanism for Group-V Precursor Dissociation on Si(001). Physical Review Letters, 2006, 97, 046103.	7.8	10
74	Dynamic formation process of Bi line structure on Si(100) surface. Computational Materials Science, 2006, 36, 135-138.	3.0	0
75	Adsorption, diffusion, and site exchange for Ge ad-dimers on Sb-covered Si(001) from first-principles total-energy calculations. Physical Review B, 2006, 74, .	3.2	7
76	First-Principles Study of the Electronic Properties of γ and γ' Interface in Ni Based Superalloys. Materials Transactions, 2005, 46, 1122-1126.	1.2	1
77	Dynamic Ad-Dimer Twisting Assisted Nanowire Self-Assembly on Si(001). Physical Review Letters, 2005, 94, 226103.	7.8	21
78	Molecular orbital analysis of frontier orbitals for molecular electronics: a case study of unimolecular rectifier and photovoltaic cell. Science and Technology of Advanced Materials, 2003, 4, 377-382.	6.1	8
79	Stability of Sb line structures on Si(001). Physical Review B, 2003, 67, .	3.2	17
80	Ab initio Monte Carlo Studies on Magnetic Properties of Tetragonal L1 ₀ Ordered 3d/Au Superlattices. Materials Transactions, 2003, 44, 1529-1534.	1.2	5
81	First-principles studies on the structural and magnetic properties of (Cr, Mn, Fe)/Ag monatomic multilayers. Journal of Physics Condensed Matter, 1998, 10, 9655-9662.	1.8	10
82	La induced Si ₃ trimer monolayer on Si(111) surface: An ab initio study. New Journal of Physics, 0, .	2.9	1