Chaoyu He

List of Publications by Year in descending order

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83 papers	2,151 citations	201674 27 h-index	243625 44 g-index
83 all docs	83 docs citations	83 times ranked	2131 citing authors

#	Article	IF	Citations
1	Magnetic Properties of Single Transition-Metal Atom Absorbed Graphdiyne and Graphyne Sheet from DFT+U Calculations. Journal of Physical Chemistry C, 2012, 116, 26313-26321.	3.1	264
2	Stochastic generation of complex crystal structures combining group and graph theory with application to carbon. Physical Review B, 2018, 97, .	3.2	114
3	Complex Low Energy Tetrahedral Polymorphs of Group IV Elements from First Principles. Physical Review Letters, 2018, 121, 175701.	7.8	95
4	Stone-Wales graphene: A two-dimensional carbon semimetal with magic stability. Physical Review B, 2019, 99, .	3.2	95
5	Thermal and thermoelectric properties of monolayer indium triphosphide (InP₃): a first-principles study. Journal of Materials Chemistry A, 2018, 6, 21532-21541.	10.3	91
6	New superhard carbon phases between graphite and diamond. Solid State Communications, 2012, 152, 1560-1563.	1.9	89
7	Z-BN: a novel superhard boron nitride phase. Physical Chemistry Chemical Physics, 2012, 14, 10967.	2.8	72
8	Four superhard carbon allotropes: a first-principles study. Physical Chemistry Chemical Physics, 2012, 14, 8410.	2.8	66
9	Lattice thermal conductivity of borophene from first principle calculation. Scientific Reports, 2017, 7, 45986.	3.3	60
10	A novel WS₂/NbSe₂ vdW heterostructure as an ultrafast charging and discharging anode material for lithium-ion batteries. Journal of Materials Chemistry A, 2018, 6, 17040-17048.	10.3	53
11	Theoretical prediction of low-energy Stone-Wales graphene with an intrinsic type-III Dirac cone. Physical Review B, 2020, 101, .	3.2	53
12	Two-dimensional topological insulators with tunable band gaps: Single-layer HgTe and HgSe. Scientific Reports, 2015, 5, 14115.	3.3	50
13	Direct and quasi-direct band gap silicon allotropes with remarkable stability. Physical Chemistry Chemical Physics, 2016, 18, 9682-9686.	2.8	49
14	Two viable three-dimensional carbon semiconductors with an entirely sp²configuration. Physical Chemistry Chemical Physics, 2013, 15, 680-684.	2.8	48
15	Stability of two-dimensional PN monolayer sheets and their electronic properties. Physical Chemistry Chemical Physics, 2015, 17, 32009-32015.	2.8	47
16	Structure, stability and electronic properties of tricycle type graphane. Physica Status Solidi - Rapid Research Letters, 2012, 6, 427-429.	2.4	43
17	Two-Dimensional Carbon Allotropes and Nanoribbons based on 2,6-Polyazulene Chains: Stacking Stabilities and Electronic Properties. Journal of Physical Chemistry Letters, 2021, 12, 732-738.	4.6	41
18	Strain engineering the structures and electronic properties of Janus monolayer transition-metal dichalcogenides. Journal of Applied Physics, 2019, 125, .	2.5	39

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19	Si-Cmma: A silicon thin film with excellent stability and Dirac nodal loop. Physical Review B, 2019, 100, .	3.2	36
20	Density functional theory study of Fe adatoms adsorbed monolayer and bilayer MoS2 sheets. Journal of Applied Physics, 2013, 114, .	2.5	35
21	High-Throughput Screening of Two-Dimensional Planar sp² Carbon Space Associated with a Labeled Quotient Graph. Journal of Physical Chemistry Letters, 2021, 12, 11511-11519.	4.6	34
22	The structural, electronic and magnetic properties of bi-layered MoS2 with transition-metals doped in the interlayer. RSC Advances, 2013, 3, 12939.	3.6	33
23	Newly discovered graphyne allotrope with rare and robust Dirac node loop. Nanoscale, 2021, 13, 3564-3571.	5.6	33
24	Five low energy phosphorene allotropes constructed through gene segments recombination. Scientific Reports, 2017, 7, 46431.	3.3	31
25	Intrinsic piezoelectricity of monolayer group IVâ€“V MX2: SiP2, SiAs2, GeP2, and GeAs2. Applied Physics Letters, 2020, 116, .	3.3	30
26	Firstâ€principles prediction of a novel hexagonal phosphorene allotrope. Physica Status Solidi - Rapid Research Letters, 2016, 10, 563-565.	2.4	28
27	New candidate for the simple cubic carbon sample shock-synthesized by compression of the mixture of carbon black and tetracyanoethylene. Carbon, 2017, 112, 91-96.	10.3	27
28	New Two-Dimensional Wide Band Gap Hydrocarbon Insulator by Hydrogenation of a Biphenylene Sheet. Journal of Physical Chemistry Letters, 2021, 12, 8889-8896.	4.6	26
29	The intrinsic thermal transport properties of the biphenylene network and the influence of hydrogenation: a first-principles study. Journal of Materials Chemistry C, 2021, 9, 16945-16951.	5.5	26
30	M585, a low energy superhard monoclinic carbon phase. Solid State Communications, 2014, 181, 24-27.	1.9	25
31	Bayesian optimization-based design of defect gamma-graphyne nanoribbons with high thermoelectric conversion efficiency. Carbon, 2021, 176, 52-60.	10.3	25
32	Modulation effect of hydrogen and fluorine decoration on the surface work function of BN sheets. AIP Advances, 2012, 2, .	1.3	18
33	Structures, stability, mechanical and electronic properties of Î±-boron andÎ±*-boron. AIP Advances, 2013, 3, .	1.3	18
34	Tunable photoelectronic properties of hydrogenated-silicene/halogenated-silicene superlattices for water splitting. Journal of Applied Physics, 2020, 127, .	2.5	18
35	Ge3P2: New viable two-dimensional semiconductors with ultrahigh carrier mobility. Applied Surface Science, 2019, 497, 143803.	6.1	17
36	Systematic Enumeration of Lowâ€Energy Graphyne Allotropes Based on a Coordinationâ€Constrained Searching Strategy. Physica Status Solidi - Rapid Research Letters, 2020, 14, 2000437.	2.4	17

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37	Allotropes of Phosphorus with Remarkable Stability and Intrinsic Piezoelectricity. Physical Review Applied, 2018, 9, .	3.8	16
38	Robust transport of charge carriers in in-plane 1Tâ€²-2H MoTe2 homojunctions with ohmic contact. Nano Research, 2021, 14, 1311-1318.	10.4	16
39	Potential thermoelectric material open framework Si24 from a first-principles study. Journal Physics D: Applied Physics, 2017, 50, 425501.	2.8	15
40	The thermoelectric properties of monolayer SiP and GeP from first-principles calculations. Journal of Applied Physics, 2019, 126, .	2.5	14
41	Photogalvanicâ€Effectâ€Induced Spinâ€Polarized Current in Defective Silicane with H Vacancies. Physica Status Solidi - Rapid Research Letters, 2020, 14, 2000395.	2.4	13
42	Lowâ€Energy GeP Monolayers with Natural Typeâ€II Homojunctions for SunLightâ€Driven Water Splitting. Physica Status Solidi - Rapid Research Letters, 2019, 13, 1900470.	2.4	12
43	First-principles prediction of three new graphitic C3N4 allotropes with potentials for application in sun-light-driven water splitting. Physica B: Condensed Matter, 2019, 562, 131-134.	2.7	12
44	Optoelectronic properties of type-II SePtTe/InS van der Waals heterojunction. Journal of Applied Physics, 2020, 128, .	2.5	12
45	Surface oxidation: an effective way to induce piezoelectricity in 2D black phosphorus. Journal Physics D: Applied Physics, 2018, 51, 12LT01.	2.8	11
46	Low energy three-dimensional hydrocarbon crystal from cold compression of benzene. Journal of Physics Condensed Matter, 2013, 25, 205403.	1.8	10
47	First-principles prediction of two hexagonal silicon crystals as potential absorbing layer materials for solar-cell application. Journal of Applied Physics, 2018, 124, .	2.5	10
48	Potential thermoelectric candidate monolayer silicon diphosphide (SiP2) from a first-principles calculation. Computational Materials Science, 2021, 188, 110154.	3.0	10
49	SIn₂Te/TeIn₂Se: a type-II heterojunction as a water-splitting photocatalyst with high solar energy harvesting. Journal of Materials Chemistry C, 2021, 9, 7734-7744.	5.5	10
50	Ab initioprediction of a new allotrope of two-dimensional silicon. Physica Status Solidi - Rapid Research Letters, 2017, 11, 1600422.	2.4	9
51	Transport Properties of Zigzag Graphene Nanoribbons Decorated by Carboxyl Group Chains. Journal of Physical Chemistry C, 2011, 115, 21893-21898.	3.1	8
52	Strain effects on magnetic states of monolayer MoS2 doped with group IIIA to VA atoms. Physica E: Low-Dimensional Systems and Nanostructures, 2019, 114, 113609.	2.7	8
53	Few-Layer <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" overflow="scroll"><mml:mi>Î²</mml:mi></mml:math> - <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" overflow="scroll"><mml:mrow><mml:mi>Sn</mml:mi><mml:mi>Se</mml:mi></mml:mrow></mml:math> with Strong Visible Light Absorbance and Ultrahigh Carrier Mobility. Physical Review Applied, 2020, 13, .	3.8	8
54	Notable effect of magnetic order on the phonon transport in semi-hydrogenated graphene. Applied Physics Letters, 2022, 120, .	3.3	8

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55	Thermoelectric properties of four typical silicon allotropes. Modelling and Simulation in Materials Science and Engineering, 2018, 26, 085006.	2.0	7
56	First-principles prediction of two atomic-thin phosphorene allotropes with potentials for sun-light-driven water splitting. Journal of Physics Condensed Matter, 2019, 31, 075702.	1.8	7
57	Strain effect on phonon transport in open framework Si24: A first-principles study. Physica E: Low-Dimensional Systems and Nanostructures, 2020, 118, 113870.	2.7	7
58	Dirac Semimetal Protected by Nonsymmorphic Mirror Symmetries in TPHâ€Graphene. Physica Status Solidi - Rapid Research Letters, 2021, 15, 2100039.	2.4	7
59	Type-II lateral SnSe/GeTe heterostructures for solar photovoltaic applications with high efficiency. Nanoscale Advances, 2021, 3, 3643-3649.	4.6	7
60	Doping Induced Abnormal Contraction and Significant Reduction of Lattice Thermal Conductivity of Open Framework Si24. ES Energy & Environments, 2018, , .	1.1	7
61	First-principles study on the electronic, mechanical and optical properties for silicon allotropes in hexagonal 2â€“7 stacking orders. Scripta Materialia, 2022, 219, 114843.	5.2	7
62	First-principles study of the structures and fundamental electronic properties of two-dimensional P_{0.5}As_{0.5}alloy. Physica Status Solidi (B): Basic Research, 2017, 254, 1700157.	1.5	6
63	Band offsets engineering in asymmetric Janus bilayer transition-metal dichalcogenides. Journal of Physics Condensed Matter, 2020, 32, 035502.	1.8	6
64	Optimizing the thermoelectric performance of graphyne nanotube via applying radial strain. Journal of Applied Physics, 2017, 121, 125112.	2.5	5
65	First-principles study of magnetic properties of ultra-thin MoSi2 films. Journal of Applied Physics, 2018, 123, 104304.	2.5	5
66	Effects of contact oxidization on the transport properties of Au/ZGNR junctions. Physica Status Solidi - Rapid Research Letters, 2012, 6, 457-459.	2.4	4
67	Effect of hydrogen passivation on the decoupling of graphene on SiC(0001) substrate: First-principles calculations. Scientific Reports, 2017, 7, 8461.	3.3	4
68	Tunable topologically nontrivial states in newly discovered graphyne allotropes: from Dirac nodal grid to Dirac nodal loop. Nanotechnology, 2021, 32, 485705.	2.6	4
69	Electronic and Spinâ€Dependent Optical Properties of Feâ€Adsorbed Armchair Silicene/Silicane Superlattices. Physica Status Solidi - Rapid Research Letters, 2020, 14, 1900494.	2.4	3
70	Quasi-bonding driven abnormal isotropic thermal transport in intrinsically anisotropic nanostructure: a case of study of a phosphorus nanotube array. Nanotechnology, 2020, 31, 095704.	2.6	3
71	Hydrogenated graphene: Structures and surface work function. , 2012, , .		2
72	Geometries and Electronic Properties of Black Phosphorus/MoS2 Heterostructure with P Atom Vacancies: First Principles Calculations. Journal of Electronic Materials, 2020, 49, 5730-5738.	2.2	2

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73	New structure candidates for the experimentally synthesized heptazine-based and triazine-based two dimensional graphitic carbon nitride. Physica E: Low-Dimensional Systems and Nanostructures, 2021, 128, 114535.	2.7	2
74	Ferromagnetism triggered by nitrogen defects in graphitic carbon nitride. Journal Physics D: Applied Physics, 2020, 53, 495002.	2.8	2
75	Effective Fermi level tuning of Bi2Se3 by introducing CdBi/CaBi dopant. RSC Advances, 2014, 4, 10499.	3.6	1
76	Charge transport properties of graphene: Effects of Cu-based gate electrode. Journal of Applied Physics, 2016, 120, .	2.5	1
77	The thermoelectric performance of dumbbell silicene nanoribbons. Fullerenes Nanotubes and Carbon Nanostructures, 2018, 26, 511-517.	2.1	1
78	First-principles prediction of a new ground state for surface-oxidized phosphorene with remarkable piezoelectricity. Journal Physics D: Applied Physics, 2019, 52, 295301.	2.8	1
79	Excellent thermoelectric performance of open framework Si24 nanowires from density functional based tight-binding calculation. Journal of Applied Physics, 2020, 128, 215108.	2.5	1
80	Strain induced magnetic hysteresis in MoS₂ and WS₂ monolayers with symmetric double sulfur vacancy defects. Physical Chemistry Chemical Physics, 2022, 24, 17263-17270.	2.8	1
81	Structures, stability and electronic properties of two- or four-segment BN/C nanotubes. , 2012, , .		0
82	Enhanced and spin-dependent infrared optical response of silicene/silicane superlattices with Cr adsorption. Journal Physics D: Applied Physics, 2021, 54, 405106.	2.8	0
83	KP15: Natural van der Waals material with ultra-low thermal conductivity and excellent thermoelectric performance. Journal of Applied Physics, 2021, 130, 195104.	2.5	0