Chunxiao Zhang

List of Publications by Year
in descending order

69 papers	1,582 citations	304743 22 h-index	315739 38 g-index
69 all docs	69 docs citations	69 times ranked	1698 citing authors

#	Article	IF	Citations
1	Notable effect of magnetic order on the phonon transport in semi-hydrogenated graphene. Applied Physics Letters, 2022, 120, .	3.3	8
2	Potential thermoelectric candidate monolayer silicon diphosphide (SiP2) from a first-principles calculation. Computational Materials Science, 2021, 188, 110154.	3.0	10
3	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
4	Newly discovered graphyne allotrope with rare and robust Dirac node loop. Nanoscale, 2021, 13, 3564-3571.	5.6	33
5	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
6	Bayesian optimization-based design of defect gamma-graphyne nanoribbons with high thermoelectric conversion efficiency. Carbon, 2021, 176, 52-60.	10.3	25
7	Effects of Charge Transfer on the Critical Distance of the Interlayer Ferromagnetic Order Transition in SCrSeâ€Based van der Waals Bilayers. Physica Status Solidi - Rapid Research Letters, 2021, 15, 2100213.	2.4	0
8	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
9	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
10	Tunable topologically nontrivial states in newly discovered graphyne allotropes: from Dirac nodal grid to Dirac nodal loop. Nanotechnology, 2021, 32, 485705.	2.6	4
11	Type-II vdW heterojunction SeGa2Te/SeIn2Se as a high-efficiency visible-light-driven water-splitting photocatalyst. Physics Letters, Section A: General, Atomic and Solid State Physics, 2021, 413, 127594.	2.1	9
12	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
13	Type-II lateral SnSe/GeTe heterostructures for solar photovoltaic applications with high efficiency. Nanoscale Advances, 2021, 3, 3643-3649.	4.6	7
14	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
15	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
16	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
17	2D O-PTl monolayer: a robust large bandgap topological insulator. Journal Physics D: Applied Physics, 2020, 53, 025302.	2.8	4
18	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

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19	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
20	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
21	Photogalvanicâ€Effectâ€Induced Spinâ€Polarized Current in Defective Silicane with H Vacancies. Physica Status Solidi - Rapid Research Letters, 2020, 14, 2000395.	2.4	13
22	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
23	Optoelectronic properties of type-II SePtTe/InS van der Waals heterojunction. Journal of Applied Physics, 2020, 128, .	2.5	12
24	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
25	Excellent properties of type-II van der Waals Janus-XM2Xâ€™/MX heterojunctions toward solar cell utilization. Journal Physics D: Applied Physics, 2020, 53, 405101.	2.8	5
26	Tunable photoelectronic properties of hydrogenated-silicene/halogenated-silicene superlattices for water splitting. Journal of Applied Physics, 2020, 127, .	2.5	18
27	Intrinsic piezoelectricity of monolayer group IVâ€“V MX2: SiP2, SiAs2, GeP2, and GeAs2. Applied Physics Letters, 2020, 116, .	3.3	30
28	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
29	Theoretical prediction of low-energy Stone-Wales graphene with an intrinsic type-III Dirac cone. Physical Review B, 2020, 101, .	3.2	53
30	Ferromagnetism triggered by nitrogen defects in graphitic carbon nitride. Journal Physics D: Applied Physics, 2020, 53, 495002.	2.8	2
31	A comparative investigation of metal (Li, Ca and Sc)-decorated 6,6,12-graphyne monolayers and 6,6,12-graphyne nanotubes for hydrogen storage. Applied Surface Science, 2019, 498, 143763.	6.1	20
32	Ge3P2: New viable two-dimensional semiconductors with ultrahigh carrier mobility. Applied Surface Science, 2019, 497, 143803.	6.1	17
33	Stone-Wales graphene: A two-dimensional carbon semimetal with magic stability. Physical Review B, 2019, 99, .	3.2	95
34	First principles study of semihydrogenated graphene and topological insulator heterojunction. Journal of Physics Condensed Matter, 2019, 31, 365002.	1.8	5
35	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
36	The thermoelectric properties of monolayer SiP and GeP from first-principles calculations. Journal of Applied Physics, 2019, 126, .	2.5	14

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37	Allotropes of Phosphorus with Remarkable Stability and Intrinsic Piezoelectricity. Physical Review Applied, 2018, 9, .	3.8	16
38	Modulation of magnetism in transition-metal-doped two-dimensional GeS. Journal Physics D: Applied Physics, 2018, 51, 225001.	2.8	2
39	Prediction of two-dimensional nodal-line semimetals in a carbon nitride covalent network. Journal of Materials Chemistry A, 2018, 6, 11252-11259.	10.3	101
40	Thermoelectric properties of four typical silicon allotropes. Modelling and Simulation in Materials Science and Engineering, 2018, 26, 085006.	2.0	7
41	Complex Low Energy Tetrahedral Polymorphs of Group IV Elements from First Principles. Physical Review Letters, 2018, 121, 175701.	7.8	95
42	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
43	Band gap reduction in van der Waals layered 2D materials via a de-charge transfer mechanism. Nanoscale, 2018, 10, 16759-16764.	5.6	25
44	Stability and magnetic properties of SnSe monolayer doped by transition metal atom (Mn, Fe, and Co): a first-principles study. Journal Physics D: Applied Physics, 2018, 51, 245004.	2.8	18
45	Doping Induced Abnormal Contraction and Significant Reduction of Lattice Thermal Conductivity of Open Framework Si24. ES Energy & Environments, 2018, , .	1.1	7
46	Ab initioprediction of a new allotrope of two-dimensional silicon. Physica Status Solidi - Rapid Research Letters, 2017, 11, 1600422.	2.4	9
47	Five low energy phosphorene allotropes constructed through gene segments recombination. Scientific Reports, 2017, 7, 46431.	3.3	31
48	Optimizing the thermoelectric performance of graphyne nanotube via applying radial strain. Journal of Applied Physics, 2017, 121, 125112.	2.5	5
49	Effect of hydrogen passivation on the decoupling of graphene on SiC(0001) substrate: First-principles calculations. Scientific Reports, 2017, 7, 8461.	3.3	4
50	Firstâ€principles prediction of a novel hexagonal phosphorene allotrope. Physica Status Solidi - Rapid Research Letters, 2016, 10, 563-565.	2.4	28
51	Charge transport properties of graphene: Effects of Cu-based gate electrode. Journal of Applied Physics, 2016, 120, .	2.5	1
52	Strain engineering of magnetic state in vacancy-doped phosphorene. Physics Letters, Section A: General, Atomic and Solid State Physics, 2016, 380, 3270-3277.	2.1	26
53	Direct and quasi-direct band gap silicon allotropes with remarkable stability. Physical Chemistry Chemical Physics, 2016, 18, 9682-9686.	2.8	49
54	Spin Switch of the Transition-Metal-Doped Boron Nitride Sheet through H/F Chemical Decoration. Journal of Physical Chemistry C, 2014, 118, 8899-8906.	3.1	27

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55	First-principles study of native point defects in Bi2Se3. AIP Advances, 2013, 3, .	1.3	73
56	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
57	Modulation effect of hydrogen and fluorine decoration on the surface work function of BN sheets. AIP Advances, 2012, 2, .	1.3	18
58	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
59	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
60	Structures, stability and electronic properties of two- or four-segment BN/C nanotubes. , 2012, , .		0
61	Structure, stability and electronic properties of tricycle type graphane. Physica Status Solidi - Rapid Research Letters, 2012, 6, 427-429.	2.4	43
62	Transport properties of hybrid graphene/graphane nanoribbons. Applied Physics Letters, 2012, 100, 103109.	3.3	10
63	Hydrogenated graphene: Structures and surface work function. , 2012, , .		2
64	Transport Properties of Zigzag Graphene Nanoribbons Decorated by Carboxyl Group Chains. Journal of Physical Chemistry C, 2011, 115, 21893-21898.	3.1	8
65	Transport Properties of Hybrid Zigzag Graphene and Boron Nitride Nanoribbons. Journal of Physical Chemistry C, 2011, 115, 10836-10841.	3.1	45
66	Electronic structures and optical properties of hexagonal boron nitride under hydrostatic pressures. Journal of Applied Physics, 2011, 109, 073708.	2.5	14
67	Transport properties of corrugated graphene nanoribbons. Applied Physics Letters, 2010, 96, .	3.3	33
68	Excellent thermoelectric performance is predicted in Sb2Te with natural superlattice structure. Chinese Physics B, 0, , .	1.4	0
69	Giant Rashba Spin Splitting in Sb/Bi2Se3/Sb and Sb/Sb2Te3 /Sb Heterojunctions. Journal of Electronic Materials, 0, , .	2.2	0