Minglei Sun

List of Publications by Year
in descending order

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72 papers	5,277 citations	46918 47 h-index	85405 71 g-index
72 all docs	72 docs citations	72 times ranked	2943 citing authors

#	Article	IF	Citations
1	MoS₂/ZnO van der Waals heterostructure as a high-efficiency water splitting photocatalyst: a first-principles study. Physical Chemistry Chemical Physics, 2018, 20, 13394-13399.	1.3	292
2	Electronic properties of blue phosphorene/graphene and blue phosphorene/graphene-like gallium nitride heterostructures. Physical Chemistry Chemical Physics, 2017, 19, 17324-17330.	1.3	180
3	Electronic and optical properties of van der Waals heterostructures of g-GaN and transition metal dichalcogenides. Applied Surface Science, 2019, 492, 513-519.	3.1	178
4	Electronic and optical properties of heterostructures based on transition metal dichalcogenides and graphene-like zinc oxide. Scientific Reports, 2018, 8, 12009.	1.6	173
5	Tunable Schottky barrier in van der Waals heterostructures of graphene and g-GaN. Applied Physics Letters, 2017, 110, .	1.5	166
6	Direct Pyrolysis of Supermolecules: An Ultrahigh Edgeâ€Nitrogen Doping Strategy of Carbon Anodes for Potassiumâ€Ion Batteries. Advanced Materials, 2020, 32, e2000732.	11.1	164
7	First-principle study of electronic and optical properties of two-dimensional materials-based heterostructures based on transition metal dichalcogenides and boron phosphide. Applied Surface Science, 2019, 476, 70-75.	3.1	154
8	B₂P₆: A Two-Dimensional Anisotropic Janus Material with Potential in Photocatalytic Water Splitting and Metal-Ion Batteries. Chemistry of Materials, 2020, 32, 4795-4800.	3.2	142
9	Electronic and magnetic properties of 4d series transition metal substituted graphene: A first-principles study. Carbon, 2017, 120, 265-273.	5.4	135
10	Effects of structural imperfection on the electronic properties of graphene/WSe₂ heterostructures. Journal of Materials Chemistry C, 2017, 5, 10383-10390.	2.7	131
11	A first principles investigation on the structural, mechanical, electronic, and catalytic properties of biphenylene. Scientific Reports, 2021, 11, 19008.	1.6	124
12	Structure Prototype Outperforming MXenes in Stability and Performance in Metalâ€Ion Batteries: A High Throughput Study. Advanced Energy Materials, 2021, 11, 2003633.	10.2	111
13	First-Principles Study on Transition-Metal Dichalcogenide/BSe van der Waals Heterostructures: A Promising Water-Splitting Photocatalyst. Journal of Physical Chemistry C, 2019, 123, 22742-22751.	1.5	110
14	High-efficiency photocatalyst for water splitting: a Janus MoSSe/XN (Xâ€‰â€‰=â€‰â€‰Ga, Al) van der Waals heterostructure. Journal Physics D: Applied Physics, 2020, 53, 185504.	1.3	110
15	A direct Z-scheme PtS₂/arsenene van der Waals heterostructure with high photocatalytic water splitting efficiency. Nanoscale, 2020, 12, 17281-17289.	2.8	108
16	Exceptional Optical Absorption of Buckled Arsenene Covering a Broad Spectral Range by Molecular Doping. ACS Omega, 2018, 3, 8514-8520.	1.6	107
17	Transition-metal dichalcogenides/Mg(OH)₂ van der Waals heterostructures as promising water-splitting photocatalysts: a first-principles study. Physical Chemistry Chemical Physics, 2019, 21, 1791-1796.	1.3	106
18	Ultrahigh Carrier Mobility in the Two-Dimensional Semiconductors B₈Si₄, B₈Ge₄, and B₈Sn₄. Chemistry of Materials, 2021, 33, 6475-6483.	3.2	104

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19	Transition metal doped arsenene: A first-principles study. Applied Surface Science, 2016, 389, 594-600.	3.1	102
20	A first-principles study of light non-metallic atom substituted blue phosphorene. Applied Surface Science, 2015, 356, 110-114.	3.1	95
21	First-principles study of the alkali earth metal atoms adsorption on graphene. Applied Surface Science, 2015, 356, 668-673.	3.1	90
22	AccordionâEŁike Carbon with High Nitrogen Doping for Fast and Stable K Ion Storage. Advanced Energy Materials, 2021, 11, 2101928.	10.2	88
23	Few-Layer PdSe₂ Sheets: Promising Thermoelectric Materials Driven by High Valley Convergence. ACS Omega, 2018, 3, 5971-5979.	1.6	87
24	Point Defects in Blue Phosphorene. Chemistry of Materials, 2019, 31, 8129-8135.	3.2	86
25	Strain-enhanced properties of van der Waals heterostructure based on blue phosphorus and g-GaN as a visible-light-driven photocatalyst for water splitting. RSC Advances, 2019, 9, 4816-4823.	1.7	86
26	Magnetism in non-metal atoms adsorbed graphene-like gallium nitride monolayers. Applied Surface Science, 2018, 427, 609-612.	3.1	79
27	Alkali-metal-adsorbed g-GaN monolayer: ultralow work functions and optical properties. Nanoscale Research Letters, 2018, 13, 207.	3.1	79
28	Adsorption of Transition Metals on Black Phosphorene: a First-Principles Study. Nanoscale Research Letters, 2018, 13, 282.	3.1	79
29	A van der Waals Heterostructure Based on Graphene-like Gallium Nitride and Boron Selenide: A High-Efficiency Photocatalyst for Water Splitting. ACS Omega, 2019, 4, 21689-21697.	1.6	78
30	Beryllene: A Promising Anode Material for Na- and K-Ion Batteries with Ultrafast Charge/Discharge and High Specific Capacity. Journal of Physical Chemistry Letters, 2020, 11, 9051-9056.	2.1	78
31	First-principles calculations of the electronic properties of SiC-based bilayer and trilayer heterostructures. Physical Chemistry Chemical Physics, 2018, 20, 24726-24734.	1.3	77
32	Theoretical Study of GaN/BP van der Waals Nanocomposites with Strain-Enhanced Electronic and Optical Properties for Optoelectronic Applications. ACS Applied Nano Materials, 2019, 2, 6482-6491.	2.4	75
33	Tuning electronic and magnetic properties of blue phosphorene by doping Al, Si, As and Sb atom: A DFT calculation. Solid State Communications, 2016, 242, 36-40.	0.9	72
34	Magnetism in transition-metal-doped germanene: A first-principles study. Computational Materials Science, 2016, 118, 112-116.	1.4	69
35	Î´-CS: A Direct-Band-Gap Semiconductor Combining Auxeticity, Ferroelasticity, and Potential for High-Efficiency Solar Cells. Physical Review Applied, 2020, 14, .	1.5	69
36	Enhancing electronic and optical properties of monolayer MoSe₂via a MoSe₂/blue phosphorene heterobilayer. Physical Chemistry Chemical Physics, 2019, 21, 15760-15766.	1.3	68

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37	Using van der Waals heterostructures based on two-dimensional blue phosphorus and XC (X = Ge, Si) for water-splitting photocatalysis: a first-principles study. Physical Chemistry Chemical Physics, 2019, 21, 9949-9956.	1.3	66
38	Hydrogenated and halogenated blue phosphorene as Dirac materials: A first principles study. Applied Surface Science, 2017, 392, 46-50.	3.1	64
39	First principles study of silicene symmetrically and asymmetrically functionalized with halogen atoms. RSC Advances, 2016, 6, 95846-95854.	1.7	63
40	Graphene-Oxide-Assisted Synthesis of Ga₂O₃ Nanosheets/Reduced Graphene Oxide Nanocomposites Anodes for Advanced Alkali-Ion Batteries. ACS Applied Energy Materials, 2018, 1, 4708-4715.	2.5	61
41	Electronic and optical properties of van der Waals vertical heterostructures based on two-dimensional transition metal dichalcogenides: First-principles calculations. Physics Letters, Section A: General, Atomic and Solid State Physics, 2019, 383, 1487-1492.	0.9	60
42	Pd₄S₃Se₃, Pd₄S₃Te₃, and Pd₄Se₃Te₃: Candidate Two-Dimensional Janus Materials for Photocatalytic Water Splitting. Chemistry of Materials, 2021, 33, 4128-4134.	3.2	59
43	Electronic and magnetic behaviors of graphene with 5d series transition metal atom substitutions: A first-principles study. Physica E: Low-Dimensional Systems and Nanostructures, 2016, 80, 142-148.	1.3	56
44	A MoSSe/blue phosphorene vdw heterostructure with energy conversion efficiency of 19.9% for photocatalytic water splitting. Semiconductor Science and Technology, 2020, 35, 125008.	1.0	56
45	Transition metal doped puckered arsenene: Magnetic properties and potential as a catalyst. Physica E: Low-Dimensional Systems and Nanostructures, 2019, 108, 153-159.	1.3	55
46	Electronic properties of Janus silicene: new direct band gap semiconductors. Journal Physics D: Applied Physics, 2016, 49, 445305.	1.3	51
47	Rational design of carbon anodes by catalytic pyrolysis of graphitic carbon nitride for efficient storage of Na and K mobile ions. Nano Energy, 2021, 87, 106184.	8.2	50
48	Halogenated arsenenes as Dirac materials. Applied Surface Science, 2016, 376, 286-289.	3.1	49
49	Lowâ€Symmetry PdSe₂ for High Performance Thermoelectric Applications. Advanced Functional Materials, 2020, 30, 2004896.	7.8	49
50	Tunable Schottky barrier in graphene/graphene-like germanium carbide van der Waals heterostructure. Scientific Reports, 2019, 9, 5208.	1.6	48
51	Magnetism in transition metal-substituted germanane: A search for room temperature spintronic devices. Journal of Applied Physics, 2016, 119, .	1.1	46
52	Weak Câ€“Hâ‹¯Fâ€“C hydrogen bonds make a big difference in graphane/fluorographane and fluorographene/fluorographane bilayers. Physical Chemistry Chemical Physics, 2017, 19, 28127-28132.	1.3	41
53	A Cyclized Polyacrylonitrile Anode for Alkali Metal Ion Batteries. Angewandte Chemie - International Edition, 2021, 60, 1355-1363.	7.2	41
54	Unique Omnidirectional Negative Poissonâ€™s Ratio in Î´-Phase Carbon Monochalcogenides. Journal of Physical Chemistry C, 2021, 125, 4133-4138.	1.5	39

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55	First-principles calculations of aluminium nitride monolayer with chemical functionalization. Applied Surface Science, 2019, 481, 1549-1553.	3.1	36
56	Study on structural, electronic and magnetic properties of Sn atom adsorbed on defective graphene by first-principle calculations. Applied Surface Science, 2014, 307, 158-164.	3.1	29
57	Valley Hall Effect and Magnetic Moment in Magnetized Silicene. Journal of Superconductivity and Novel Magnetism, 2019, 32, 2947-2957.	0.8	28
58	Oxygenated (113) diamond surface for nitrogen-vacancy quantum sensors with preferential alignment and long coherence time from first principles. Carbon, 2019, 145, 273-280.	5.4	24
59	Spin and valley filter across line defect in silicene. Applied Physics Express, 2018, 11, 053004.	1.1	23
60	First-principles investigation on electronic properties and band alignment of group III monochalcogenides. Scientific Reports, 2019, 9, 13289.	1.6	23
61	Protected valley states and generation of valley- and spin-polarized current in monolayer <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mrow><mml:mi>M</mml:mi> Physical Review B, 2022, 105, .	1.1	21
62	Chiral filtration-induced spin/valley polarization in silicene line defects. Applied Physics Express, 2018, 11, 063006.	1.1	15
63	Two-Dimensional Tetrahex-GeC₂: A Material with Tunable Electronic and Optical Properties Combined with Ultrahigh Carrier Mobility. ACS Applied Materials & Interfaces, 2021, 13, 14489-14496.	4.0	15
64	Molecular doping of blue phosphorene: a first-principles investigation. Journal of Physics Condensed Matter, 2020, 32, 055501.	0.7	14
65	Enhanced photoresponse of highly air-stable palladium diselenide by thickness engineering. Nanophotonics, 2020, 9, 2467-2474.	2.9	10
66	A Cyclized Polyacrylonitrile Anode for Alkali Metal Ion Batteries. Angewandte Chemie, 2021, 133, 1375-1383.	1.6	8
67	Low-energy Ga₂O₃ polymorphs with low electron effective masses. Physical Chemistry Chemical Physics, 2022, 24, 7045-7049.	1.3	8
68	Semimetallic 2D Alkynyl Carbon Materials with Distorted Type I Dirac Cones. Journal of Physical Chemistry C, 2021, 125, 18022-18030.	1.5	7
69	Switchable metal-to-half-metal transition at the semi-hydrogenated graphene/ferroelectric interface. Nanoscale, 2020, 12, 5067-5074.	2.8	6
70	Fieldâ€Effect Transistors: Lowâ€Symmetry PdSe₂ for High Performance Thermoelectric Applications (Adv. Funct. Mater. 52/2020). Advanced Functional Materials, 2020, 30, 2070347.	7.8	3
71	Measuring the nonlocality of different types of Majorana bound states in a topological superconducting wire. Journal of Physics Condensed Matter, 2019, 31, 045501.	0.7	1
72	Manifestation of topological transitions in a multi-terminal Josephson junction. Journal of Physics Condensed Matter, 2018, 30, 385503.	0.7	0