

# Minglei Sun

## List of Publications by Citations

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70  
papers

3,318  
citations

39  
h-index

57  
g-index

72  
ext. papers

4,369  
ext. citations

6.2  
avg, IF

6.38  
L-index

#	Paper	IF	Citations
70	MoS/ZnO van der Waals heterostructure as a high-efficiency water splitting photocatalyst: a first-principles study. <i>Physical Chemistry Chemical Physics</i> , <b>2018</b> , 20, 13394-13399	3.6	200
69	Electronic properties of blue phosphorene/graphene and blue phosphorene/graphene-like gallium nitride heterostructures. <i>Physical Chemistry Chemical Physics</i> , <b>2017</b> , 19, 17324-17330	3.6	152
68	Tunable Schottky barrier in van der Waals heterostructures of graphene and g-GaN. <i>Applied Physics Letters</i> , <b>2017</b> , 110, 173105	3.4	129
67	Electronic and optical properties of van der Waals heterostructures of g-GaN and transition metal dichalcogenides. <i>Applied Surface Science</i> , <b>2019</b> , 492, 513-519	6.7	116
66	Electronic and optical properties of heterostructures based on transition metal dichalcogenides and graphene-like zinc oxide. <i>Scientific Reports</i> , <b>2018</b> , 8, 12009	4.9	110
65	Electronic and magnetic properties of 4d series transition metal substituted graphene: A first-principles study. <i>Carbon</i> , <b>2017</b> , 120, 265-273	10.4	108
64	First-principle study of electronic and optical properties of two-dimensional materials-based heterostructures based on transition metal dichalcogenides and boron phosphide. <i>Applied Surface Science</i> , <b>2019</b> , 476, 70-75	6.7	106
63	Effects of structural imperfection on the electronic properties of graphene/WSe <sub>2</sub> heterostructures. <i>Journal of Materials Chemistry C</i> , <b>2017</b> , 5, 10383-10390	7.1	105
62	B2P6: A Two-Dimensional Anisotropic Janus Material with Potential in Photocatalytic Water Splitting and Metal-Ion Batteries. <i>Chemistry of Materials</i> , <b>2020</b> , 32, 4795-4800	9.6	85
61	Transition-metal dichalcogenides/Mg(OH) van der Waals heterostructures as promising water-splitting photocatalysts: a first-principles study. <i>Physical Chemistry Chemical Physics</i> , <b>2019</b> , 21, 1791-1796	3.6	84
60	Transition metal doped arsenene: A first-principles study. <i>Applied Surface Science</i> , <b>2016</b> , 389, 594-600	6.7	82
59	A first-principles study of light non-metallic atom substituted blue phosphorene. <i>Applied Surface Science</i> , <b>2015</b> , 356, 110-114	6.7	78
58	Direct Pyrolysis of Supermolecules: An Ultrahigh Edge-Nitrogen Doping Strategy of Carbon Anodes for Potassium-Ion Batteries. <i>Advanced Materials</i> , <b>2020</b> , 32, e2000732	24	78
57	First-principles study of the alkali earth metal atoms adsorption on graphene. <i>Applied Surface Science</i> , <b>2015</b> , 356, 668-673	6.7	77
56	First-Principles Study on Transition-Metal Dichalcogenide/BSe van der Waals Heterostructures: A Promising Water-Splitting Photocatalyst. <i>Journal of Physical Chemistry C</i> , <b>2019</b> , 123, 22742-22751	3.8	73
55	Exceptional Optical Absorption of Buckled Arsenene Covering a Broad Spectral Range by Molecular Doping. <i>ACS Omega</i> , <b>2018</b> , 3, 8514-8520	3.9	73
54	High-efficiency photocatalyst for water splitting: a Janus MoSSe/XN (X = Ga, Al) van der Waals heterostructure. <i>Journal Physics D: Applied Physics</i> , <b>2020</b> , 53, 185504	3	65

53	Strain-enhanced properties of van der Waals heterostructure based on blue phosphorus and g-GaN as a visible-light-driven photocatalyst for water splitting.. <i>RSC Advances</i> , <b>2019</b> , 9, 4816-4823	3.7	62
52	Few-Layer PdSe Sheets: Promising Thermoelectric Materials Driven by High Valley Convergence. <i>ACS Omega</i> , <b>2018</b> , 3, 5971-5979	3.9	61
51	Tuning electronic and magnetic properties of blue phosphorene by doping Al, Si, As and Sb atom: A DFT calculation. <i>Solid State Communications</i> , <b>2016</b> , 242, 36-40	1.6	60
50	Point Defects in Blue Phosphorene. <i>Chemistry of Materials</i> , <b>2019</b> , 31, 8129-8135	9.6	56
49	Adsorption of Transition Metals on Black Phosphorene: a First-Principles Study. <i>Nanoscale Research Letters</i> , <b>2018</b> , 13, 282	5	56
48	Magnetism in non-metal atoms adsorbed graphene-like gallium nitride monolayers. <i>Applied Surface Science</i> , <b>2018</b> , 427, 609-612	6.7	53
47	A direct Z-scheme PtS/arsenene van der Waals heterostructure with high photocatalytic water splitting efficiency. <i>Nanoscale</i> , <b>2020</b> , 12, 17281-17289	7.7	51
46	Magnetism in transition-metal-doped germanene: A first-principles study. <i>Computational Materials Science</i> , <b>2016</b> , 118, 112-116	3.2	51
45	Hydrogenated and halogenated blue phosphorene as Dirac materials: A first principles study. <i>Applied Surface Science</i> , <b>2017</b> , 392, 46-50	6.7	51
44	A van der Waals Heterostructure Based on Graphene-like Gallium Nitride and Boron Selenide: A High-Efficiency Photocatalyst for Water Splitting. <i>ACS Omega</i> , <b>2019</b> , 4, 21689-21697	3.9	49
43	Alkali-metal-adsorbed g-GaN monolayer: ultralow work functions and optical properties. <i>Nanoscale Research Letters</i> , <b>2018</b> , 13, 207	5	49
42	Structure Prototype Outperforming MXenes in Stability and Performance in Metal-Ion Batteries: A High Throughput Study. <i>Advanced Energy Materials</i> , <b>2021</b> , 11, 2003633	21.8	48
41	First-principles calculations of the electronic properties of SiC-based bilayer and trilayer heterostructures. <i>Physical Chemistry Chemical Physics</i> , <b>2018</b> , 20, 24726-24734	3.6	46
40	Electronic and magnetic behaviors of graphene with 5d series transition metal atom substitutions: A first-principles study. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , <b>2016</b> , 80, 142-148	3	45
39	Transition metal doped puckered arsenene: Magnetic properties and potential as a catalyst. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , <b>2019</b> , 108, 153-159	3	44
38	Enhancing electronic and optical properties of monolayer MoSe via a MoSe/blue phosphorene heterobilayer. <i>Physical Chemistry Chemical Physics</i> , <b>2019</b> , 21, 15760-15766	3.6	42
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. <i>Physical Chemistry Chemical Physics</i> , <b>2019</b> , 21, 9949-9956	3.6	41
36	Electronic and optical properties of van der Waals vertical heterostructures based on two-dimensional transition metal dichalcogenides: First-principles calculations. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , <b>2019</b> , 383, 1487-1492	2.3	39

35	Halogenated arsenenes as Dirac materials. <i>Applied Surface Science</i> , <b>2016</b> , 376, 286-289	6.7	39
34	Beryllene: A Promising Anode Material for Na- and K-Ion Batteries with Ultrafast Charge/Discharge and High Specific Capacity. <i>Journal of Physical Chemistry Letters</i> , <b>2020</b> , 11, 9051-9056	6.4	39
33	First principles study of silicene symmetrically and asymmetrically functionalized with halogen atoms. <i>RSC Advances</i> , <b>2016</b> , 6, 95846-95854	3.7	39
32	Electronic properties of Janus silicene: new direct band gap semiconductors. <i>Journal Physics D: Applied Physics</i> , <b>2016</b> , 49, 445305	3	39
31	ECs: A Direct-Band-Gap Semiconductor Combining Auxeticity, Ferroelasticity, and Potential for High-Efficiency Solar Cells. <i>Physical Review Applied</i> , <b>2020</b> , 14,	4.3	38
30	Theoretical Study of GaN/BP van der Waals Nanocomposites with Strain-Enhanced Electronic and Optical Properties for Optoelectronic Applications. <i>ACS Applied Nano Materials</i> , <b>2019</b> , 2, 6482-6491	5.6	37
29	Ultrahigh Carrier Mobility in the Two-Dimensional Semiconductors B8Si4, B8Ge4, and B8Sn4. <i>Chemistry of Materials</i> , <b>2021</b> , 33, 6475-6483	9.6	37
28	Magnetism in transition metal-substituted germanane: A search for room temperature spintronic devices. <i>Journal of Applied Physics</i> , <b>2016</b> , 119, 143904	2.5	36
27	Weak C-HF-C hydrogen bonds make a big difference in graphane/fluorographane and fluorographane/fluorographane bilayers. <i>Physical Chemistry Chemical Physics</i> , <b>2017</b> , 19, 28127-28132	3.6	34
26	Graphene-Oxide-Assisted Synthesis of Ga2O3 Nanosheets/Reduced Graphene Oxide Nanocomposites Anodes for Advanced Alkali-Ion Batteries. <i>ACS Applied Energy Materials</i> , <b>2018</b> , 1, 4708-4715	6.1	34
25	A first principles investigation on the structural, mechanical, electronic, and catalytic properties of biphenylene. <i>Scientific Reports</i> , <b>2021</b> , 11, 19008	4.9	24
24	Tunable Schottky barrier in graphene/graphene-like germanium carbide van der Waals heterostructure. <i>Scientific Reports</i> , <b>2019</b> , 9, 5208	4.9	23
23	Low-Symmetry PdSe2 for High Performance Thermoelectric Applications. <i>Advanced Functional Materials</i> , <b>2020</b> , 30, 2004896	15.6	23
22	A MoSSe/blue phosphorene vdw heterostructure with energy conversion efficiency of 19.9% for photocatalytic water splitting. <i>Semiconductor Science and Technology</i> , <b>2020</b> , 35, 125008	1.8	22
21	Study on structural, electronic and magnetic properties of Sn atom adsorbed on defective graphene by first-principle calculations. <i>Applied Surface Science</i> , <b>2014</b> , 307, 158-164	6.7	21
20	Unique Omnidirectional Negative Poisson's Ratio in BPhase Carbon Monochalcogenides. <i>Journal of Physical Chemistry C</i> , <b>2021</b> , 125, 4133-4138	3.8	21
19	First-principles calculations of aluminium nitride monolayer with chemical functionalization. <i>Applied Surface Science</i> , <b>2019</b> , 481, 1549-1553	6.7	20
18	Pd4S3Se3, Pd4S3Te3, and Pd4Se3Te3: Candidate Two-Dimensional Janus Materials for Photocatalytic Water Splitting. <i>Chemistry of Materials</i> , <b>2021</b> , 33, 4128-4134	9.6	19

17	Accordion-Like Carbon with High Nitrogen Doping for Fast and Stable K Ion Storage. <i>Advanced Energy Materials</i> , <b>2021</b> , 11, 2101928	21.8	19
16	Valley Hall Effect and Magnetic Moment in Magnetized Silicene. <i>Journal of Superconductivity and Novel Magnetism</i> , <b>2019</b> , 32, 2947-2957	1.5	17
15	A Cyclized Polyacrylonitrile Anode for Alkali Metal Ion Batteries. <i>Angewandte Chemie - International Edition</i> , <b>2021</b> , 60, 1355-1363	16.4	16
14	First-principles investigation on electronic properties and band alignment of group III monochalcogenides. <i>Scientific Reports</i> , <b>2019</b> , 9, 13289	4.9	14
13	Spin and valley filter across line defect in silicene. <i>Applied Physics Express</i> , <b>2018</b> , 11, 053004	2.4	14
12	Oxygenated (113) diamond surface for nitrogen-vacancy quantum sensors with preferential alignment and long coherence time from first principles. <i>Carbon</i> , <b>2019</b> , 145, 273-280	10.4	13
11	Molecular doping of blue phosphorene: a first-principles investigation. <i>Journal of Physics Condensed Matter</i> , <b>2020</b> , 32, 055501	1.8	12
10	Chiral filtration-induced spin/valley polarization in silicene line defects. <i>Applied Physics Express</i> , <b>2018</b> , 11, 063006	2.4	10
9	Rational design of carbon anodes by catalytic pyrolysis of graphitic carbon nitride for efficient storage of Na and K mobile ions. <i>Nano Energy</i> , <b>2021</b> , 87, 106184	17.1	10
8	Enhanced photoresponse of highly air-stable palladium diselenide by thickness engineering. <i>Nanophotonics</i> , <b>2020</b> , 9, 2467-2474	6.3	6
7	Switchable metal-to-half-metal transition at the semi-hydrogenated graphene/ferroelectric interface. <i>Nanoscale</i> , <b>2020</b> , 12, 5067-5074	7.7	4
6	Two-Dimensional Tetrahex-GeC: A Material with Tunable Electronic and Optical Properties Combined with Ultrahigh Carrier Mobility. <i>ACS Applied Materials &amp; Interfaces</i> , <b>2021</b> , 13, 14489-14498	8.5	4
5	Field-Effect Transistors: Low-Symmetry PdSe <sub>2</sub> for High Performance Thermoelectric Applications (Adv. Funct. Mater. 52/2020). <i>Advanced Functional Materials</i> , <b>2020</b> , 30, 2070347	15.6	3
4	A Cyclized Polyacrylonitrile Anode for Alkali Metal Ion Batteries. <i>Angewandte Chemie</i> , <b>2021</b> , 133, 1375-1383	13.8	2
3	Manifestation of topological transitions in a multi-terminal Josephson junction. <i>Journal of Physics Condensed Matter</i> , <b>2018</b> , 30, 385503	1.8	1
2	Measuring the nonlocality of different types of Majorana bound states in a topological superconducting wire. <i>Journal of Physics Condensed Matter</i> , <b>2019</b> , 31, 045501	1.8	1
1	Semimetallic 2D Alkynyl Carbon Materials with Distorted Type I Dirac Cones. <i>Journal of Physical Chemistry C</i> , <b>2021</b> , 125, 18022-18030	3.8	1