Minglei Sun

List of Publications by Year in Descending Order

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	Structure Prototype Outperforming MXenes in Stability and Performance in Metal-Ion Batteries: A High Throughput Study. *Advanced Energy Materials*, **2021**, 11, 2003633	21.8	48
69	Two-Dimensional Tetrahex-GeC: A Material with Tunable Electronic and Optical Properties Combined with Ultrahigh Carrier Mobility. *ACS Applied Materials & Interfaces*, **2021**, 13, 14489-14496	9.5	4
68	Pd4S3Se3, Pd4S3Te3, and Pd4Se3Te3: Candidate Two-Dimensional Janus Materials for Photocatalytic Water Splitting. *Chemistry of Materials*, **2021**, 33, 4128-4134	9.6	19
67	A Cyclized Polyacrylonitrile Anode for Alkali Metal Ion Batteries. *Angewandte Chemie - International Edition*, **2021**, 60, 1355-1363	16.4	16
66	A Cyclized Polyacrylonitrile Anode for Alkali Metal Ion Batteries. *Angewandte Chemie*, **2021**, 133, 1375-1383	3.8	2
65	Unique Omnidirectional Negative Poisson□s Ratio in □Phase Carbon Monochalcogenides. *Journal of Physical Chemistry C*, **2021**, 125, 4133-4138	3.8	21
64	Ultrahigh Carrier Mobility in the Two-Dimensional Semiconductors B8Si4, B8Ge4, and B8Sn4. *Chemistry of Materials*, **2021**, 33, 6475-6483	9.6	37
63	Semimetallic 2D Alkynyl Carbon Materials with Distorted Type I Dirac Cones. *Journal of Physical Chemistry C*, **2021**, 125, 18022-18030	3.8	1
62	A first principles investigation on the structural, mechanical, electronic, and catalytic properties of biphenylene. *Scientific Reports*, **2021**, 11, 19008	4.9	24
61	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	17.1	10
60	Accordion-Like Carbon with High Nitrogen Doping for Fast and Stable K Ion Storage. *Advanced Energy Materials*, **2021**, 11, 2101928	21.8	19
59	Field-Effect Transistors: Low-Symmetry PdSe2 for High Performance Thermoelectric Applications (Adv. Funct. Mater. 52/2020). *Advanced Functional Materials*, **2020**, 30, 2070347	15.6	3
58	Direct Pyrolysis of Supermolecules: An Ultrahigh Edge-Nitrogen Doping Strategy of Carbon Anodes for Potassium-Ion Batteries. *Advanced Materials*, **2020**, 32, e2000732	24	78
57	B2P6: A Two-Dimensional Anisotropic Janus Material with Potential in Photocatalytic Water Splitting and Metal-Ion Batteries. *Chemistry of Materials*, **2020**, 32, 4795-4800	9.6	85
56	High-efficiency photocatalyst for water splitting: a Janus MoSSe/XN (X = Ga, Al) van der Waals heterostructure. *Journal Physics D: Applied Physics*, **2020**, 53, 185504	3	65
55	Enhanced photoresponse of highly air-stable palladium diselenide by thickness engineering. *Nanophotonics*, **2020**, 9, 2467-2474	6.3	6
54	A direct Z-scheme PtS/arsenene van der Waals heterostructure with high photocatalytic water splitting efficiency. *Nanoscale*, **2020**, 12, 17281-17289	7.7	51

53	Switchable metal-to-half-metal transition at the semi-hydrogenated graphene/ferroelectric interface. *Nanoscale*, **2020**, 12, 5067-5074	7.7	4
52	A MoSSe/blue phosphorene vdw heterostructure with energy conversion efficiency of 19.9% for photocatalytic water splitting. *Semiconductor Science and Technology*, **2020**, 35, 125008	1.8	22
51	Molecular doping of blue phosphorene: a first-principles investigation. *Journal of Physics Condensed Matter*, **2020**, 32, 055501	1.8	12
50	Low-Symmetry PdSe2 for High Performance Thermoelectric Applications. *Advanced Functional Materials*, **2020**, 30, 2004896	15.6	23
49	CS: A Direct-Band-Gap Semiconductor Combining Auxeticity, Ferroelasticity, and Potential for High-Efficiency Solar Cells. *Physical Review Applied*, **2020**, 14,	4.3	38
48	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	6.4	39
47	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	3.8	73
46	Point Defects in Blue Phosphorene. *Chemistry of Materials*, **2019**, 31, 8129-8135	9.6	56
45	First-principles investigation on electronic properties and band alignment of group III monochalcogenides. *Scientific Reports*, **2019**, 9, 13289	4.9	14
44	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	5.6	37
43	Oxygenated (113) diamond surface for nitrogen-vacancy quantum sensors with preferential alignment and long coherence time from first principles. *Carbon*, **2019**, 145, 273-280	10.4	13
42	First-principles calculations of aluminium nitride monolayer with chemical functionalization. *Applied Surface Science*, **2019**, 481, 1549-1553	6.7	20
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	2.3	39
40	Transition-metal dichalcogenides/Mg(OH) van der Waals heterostructures as promising water-splitting photocatalysts: a first-principles study. *Physical Chemistry Chemical Physics*, **2019**, 21, 1791-1796	3.6	84
39	Electronic and optical properties of van der Waals heterostructures of g-GaN and transition metal dichalcogenides. *Applied Surface Science*, **2019**, 492, 513-519	6.7	116
38	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	3.6	41
37	Valley Hall Effect and Magnetic Moment in Magnetized Silicene. *Journal of Superconductivity and Novel Magnetism*, **2019**, 32, 2947-2957	1.5	17
36	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	3.7	62

35	Enhancing electronic and optical properties of monolayer MoSevia a MoSe/blue phosphorene heterobilayer. *Physical Chemistry Chemical Physics*, **2019**, 21, 15760-15766	3.6	42
34	Tunable Schottky barrier in graphene/graphene-like germanium carbide van der Waals heterostructure. *Scientific Reports*, **2019**, 9, 5208	4.9	23
33	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	3.9	49
32	Transition metal doped puckered arsenene: Magnetic properties and potential as a catalyst. *Physica E: Low-Dimensional Systems and Nanostructures*, **2019**, 108, 153-159	3	44
31	Measuring the nonlocality of different types of Majorana bound states in a topological superconducting wire. *Journal of Physics Condensed Matter*, **2019**, 31, 045501	1.8	1
30	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	6.7	106
29	Spin and valley filter across line defect in silicene. *Applied Physics Express*, **2018**, 11, 053004	2.4	14
28	MoS/ZnO van der Waals heterostructure as a high-efficiency water splitting photocatalyst: a first-principles study. *Physical Chemistry Chemical Physics*, **2018**, 20, 13394-13399	3.6	200
27	Magnetism in non-metal atoms adsorbed graphene-like gallium nitride monolayers. *Applied Surface Science*, **2018**, 427, 609-612	6.7	53
26	Exceptional Optical Absorption of Buckled Arsenene Covering a Broad Spectral Range by Molecular Doping. *ACS Omega*, **2018**, 3, 8514-8520	3.9	73
25	Manifestation of topological transitions in a multi-terminal Josephson junction. *Journal of Physics Condensed Matter*, **2018**, 30, 385503	1.8	1
24	Electronic and optical properties of heterostructures based on transition metal dichalcogenides and graphene-like zinc oxide. *Scientific Reports*, **2018**, 8, 12009	4.9	110
23	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	6.1	34
22	Few-Layer PdSe Sheets: Promising Thermoelectric Materials Driven by High Valley Convergence. *ACS Omega*, **2018**, 3, 5971-5979	3.9	61
21	Alkali-metal-adsorbed g-GaN monolayer: ultralow work functions and optical properties. *Nanoscale Research Letters*, **2018**, 13, 207	5	49
20	Adsorption of Transition Metals on Black Phosphorene: a First-Principles Study. *Nanoscale Research Letters*, **2018**, 13, 282	5	56
19	First-principles calculations of the electronic properties of SiC-based bilayer and trilayer heterostructures. *Physical Chemistry Chemical Physics*, **2018**, 20, 24726-24734	3.6	46
18	Chiral filtration-induced spin/valley polarization in silicene line defects. *Applied Physics Express*, **2018**, 11, 063006	2.4	10

17	Tunable Schottky barrier in van der Waals heterostructures of graphene and g-GaN. *Applied Physics Letters*, **2017**, 110, 173105	3.4	129
16	Electronic and magnetic properties of 4d series transition metal substituted graphene: A first-principles study. *Carbon*, **2017**, 120, 265-273	10.4	108
15	Electronic properties of blue phosphorene/graphene and blue phosphorene/graphene-like gallium nitride heterostructures. *Physical Chemistry Chemical Physics*, **2017**, 19, 17324-17330	3.6	152
14	Effects of structural imperfection on the electronic properties of graphene/WSe2 heterostructures. *Journal of Materials Chemistry C*, **2017**, 5, 10383-10390	7.1	105
13	Weak C-HF-C hydrogen bonds make a big difference in graphane/fluorographane and fluorographene/fluorographane bilayers. *Physical Chemistry Chemical Physics*, **2017**, 19, 28127-28132	3.6	34
12	Hydrogenated and halogenated blue phosphorene as Dirac materials: A first principles study. *Applied Surface Science*, **2017**, 392, 46-50	6.7	51
11	Transition metal doped arsenene: A first-principles study. *Applied Surface Science*, **2016**, 389, 594-600	6.7	82
10	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	3	45
9	Halogenated arsenenes as Dirac materials. *Applied Surface Science*, **2016**, 376, 286-289	6.7	39
8	Magnetism in transition-metal-doped germanene: A first-principles study. *Computational Materials Science*, **2016**, 118, 112-116	3.2	51
7	Magnetism in transition metal-substituted germanane: A search for room temperature spintronic devices. *Journal of Applied Physics*, **2016**, 119, 143904	2.5	36
6	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	1.6	60
5	First principles study of silicene symmetrically and asymmetrically functionalized with halogen atoms. *RSC Advances*, **2016**, 6, 95846-95854	3.7	39
4	Electronic properties of Janus silicene: new direct band gap semiconductors. *Journal Physics D: Applied Physics*, **2016**, 49, 445305	3	39
3	First-principles study of the alkali earth metal atoms adsorption on graphene. *Applied Surface Science*, **2015**, 356, 668-673	6.7	77
2	A first-principles study of light non-metallic atom substituted blue phosphorene. *Applied Surface Science*, **2015**, 356, 110-114	6.7	78
1	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	6.7	21