

# Junjie He

## List of Publications by Citations

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63

papers

1,633

citations

22

h-index

39

g-index

67

ext. papers

2,116

ext. citations

6.4

avg, IF

5.28

L-index

#	Paper	IF	Citations
63	Magnetic Properties of Single Transition-Metal Atom Absorbed Graphdiyne and Graphyne Sheet from DFT+U Calculations. <i>Journal of Physical Chemistry C</i> , <b>2012</b> , 116, 26313-26321	3.8	207
62	Unusual Dirac half-metallicity with intrinsic ferromagnetism in vanadium trihalide monolayers. <i>Journal of Materials Chemistry C</i> , <b>2016</b> , 4, 2518-2526	7.1	151
61	New two-dimensional Mn-based MXenes with room-temperature ferromagnetism and half-metallicity. <i>Journal of Materials Chemistry C</i> , <b>2016</b> , 4, 11143-11149	7.1	105
60	Near-room-temperature Chern insulator and Dirac spin-gapless semiconductor: nickel chloride monolayer. <i>Nanoscale</i> , <b>2017</b> , 9, 2246-2252	7.7	88
59	High temperature spin-polarized semiconductivity with zero magnetization in two-dimensional Janus MXenes. <i>Journal of Materials Chemistry C</i> , <b>2016</b> , 4, 6500-6509	7.1	88
58	CrTiC-based double MXenes: novel 2D bipolar antiferromagnetic semiconductor with gate-controllable spin orientation toward antiferromagnetic spintronics. <i>Nanoscale</i> , <b>2018</b> , 11, 356-364	7.7	77
57	Two-dimensional honeycomb borophene oxide: strong anisotropy and nodal loop transformation. <i>Nanoscale</i> , <b>2019</b> , 11, 2468-2475	7.7	62
56	Stretch-Driven Increase in Ultrahigh Thermal Conductance of Hydrogenated Borophene and Dimensionality Crossover in Phonon Transmission. <i>Advanced Functional Materials</i> , <b>2018</b> , 28, 1801685	15.6	58
55	Twinned Growth of Metal-Free, Triazine-Based Photocatalyst Films as Mixed-Dimensional (2D/3D) van der Waals Heterostructures. <i>Advanced Materials</i> , <b>2017</b> , 29, 1703399	24	49
54	Magnetic exchange coupling and anisotropy of 3d transition metal nanowires on graphyne. <i>Scientific Reports</i> , <b>2014</b> , 4, 4014	4.9	48
53	Two-dimensional Janus transition-metal dichalcogenides with intrinsic ferromagnetism and half-metallicity. <i>Computational Materials Science</i> , <b>2018</b> , 152, 151-157	3.2	48
52	Strain control of the electronic structures, magnetic states, and magnetic anisotropy of Fe doped single-layer MoS <sub>2</sub> . <i>Computational Materials Science</i> , <b>2015</b> , 110, 102-108	3.2	41
51	Remarkably enhanced ferromagnetism in a super-exchange governed Cr <sub>2</sub> Ge <sub>2</sub> Te <sub>6</sub> monolayer via molecular adsorption. <i>Journal of Materials Chemistry C</i> , <b>2019</b> , 7, 5084-5093	7.1	32
50	Indirect-direct band gap transition through electric tuning in bilayer MoS <sub>2</sub> . <i>Journal of Chemical Physics</i> , <b>2014</b> , 140, 174707	3.9	32
49	Ni/Mo Bimetallic-Oxide-Derived Heterointerface-Rich Sulfide Nanosheets with Co-Doping for Efficient Alkaline Hydrogen Evolution by Boosting Volmer Reaction. <i>Small</i> , <b>2021</b> , 17, e2006730	11	32
48	Surfaces and morphologies of covellite (CuS) nanoparticles by means of ab initio atomistic thermodynamics. <i>CrystEngComm</i> , <b>2017</b> , 19, 3078-3084	3.3	31
47	Orbitally driven giant thermal conductance associated with abnormal strain dependence in hydrogenated graphene-like borophene. <i>Npj Computational Materials</i> , <b>2019</b> , 5,	10.9	31

46	Tailored Band Gaps in Sulfur- and Nitrogen-Containing Porous Donor-Acceptor Polymers. <i>Chemistry - A European Journal</i> , <b>2017</b> , 23, 13023-13027	4.8	30
45	Nitrogen-Doped MoS <sub>2</sub> Foam for Fast Sodium Ion Storage. <i>Advanced Materials Interfaces</i> , <b>2019</b> , 6, 19004606	4.0	28
44	Spin Switch of the Transition-Metal-Doped Boron Nitride Sheet through H/F Chemical Decoration. <i>Journal of Physical Chemistry C</i> , <b>2014</b> , 118, 8899-8906	3.8	26
43	Band Gap Engineering in an Efficient Solar-Driven Interfacial Evaporation System. <i>ACS Applied Materials &amp; Interfaces</i> , <b>2020</b> , 12, 32880-32887	9.5	23
42	Synergistically Configuring Intrinsic Activity and Fin-Tube-Like Architecture of Mn-Doped MoS <sub>2</sub> -Based Catalyst for Improved Hydrogen Evolution Reaction. <i>ACS Applied Energy Materials</i> , <b>2019</b> , 2, 493-502	6.1	23
41	Improving ionic/electronic conductivity of MoS <sub>2</sub> Li-ion anode via manganese doping and structural optimization. <i>Chemical Engineering Journal</i> , <b>2019</b> , 372, 665-672	14.7	22
40	Remarkably enhanced Curie temperature in monolayer CrI <sub>3</sub> by hydrogen and oxygen adsorption: A first-principles calculations. <i>Computational Materials Science</i> , <b>2020</b> , 183, 109820	3.2	18
39	Theoretical dissection of superconductivity in two-dimensional honeycomb borophene oxide B <sub>2</sub> O crystal with a high stability. <i>Npj Computational Materials</i> , <b>2020</b> , 6,	10.9	18
38	Low lattice thermal conductivity and promising thermoelectric figure of merit of Zintl type TlInTe <sub>2</sub> . <i>Journal of Materials Chemistry C</i> , <b>2018</b> , 6, 13269-13274	7.1	18
37	Prediction of half-semiconductor antiferromagnets with vanishing net magnetization. <i>RSC Advances</i> , <b>2015</b> , 5, 46640-46647	3.7	17
36	Direct hydrodeoxygenation of phenol over carbon-supported Ru catalysts: A computational study. <i>Journal of Molecular Catalysis A</i> , <b>2016</b> , 423, 300-307		16
35	Optically Driven Ultrafast Magnetic Order Transitions in Two-Dimensional Ferrimagnetic MXenes. <i>Journal of Physical Chemistry Letters</i> , <b>2020</b> , 11, 6219-6226	6.4	15
34	Two-dimensional MoS <sub>2</sub> -MoSe <sub>2</sub> lateral superlattice with minimized lattice thermal conductivity. <i>Journal of Applied Physics</i> , <b>2018</b> , 124, 165101	2.5	15
33	Anisotropic carrier mobility in buckled two-dimensional GaN. <i>Physical Chemistry Chemical Physics</i> , <b>2017</b> , 19, 23492-23496	3.6	14
32	Control of spintronic and electronic properties of bimetallic and vacancy-ordered vanadium carbide MXenes via surface functionalization. <i>Physical Chemistry Chemical Physics</i> , <b>2019</b> , 21, 25802-25808	3.6	14
31	The surface stability and equilibrium crystal morphology of Ni <sub>2</sub> P nanoparticles and nanowires from an ab initio atomistic thermodynamic approach. <i>CrystEngComm</i> , <b>2016</b> , 18, 3808-3818	3.3	11
30	Inartificial Two-Dimensional GeSe Janus Structures with Appropriate Direct Band Gaps and Intrinsic Polarization Boosted Charge Separation for Photocatalytic Water Splitting. <i>Journal of Physical Chemistry Letters</i> , <b>2020</b> , 11, 3095-3102	6.4	10
29	Three-dimensional graphene networks modified with acetylenic linkages for high-performance optoelectronics and Li-ion battery anode material. <i>Carbon</i> , <b>2019</b> , 154, 478-484	10.4	9

28	Low-Energy GeP Monolayers with Natural Type-II Homojunctions for SunLight-Driven Water Splitting. <i>Physica Status Solidi - Rapid Research Letters</i> , <b>2019</b> , 13, 1900470	2.5	9
27	Unravelling Photoinduced Interlayer Spin Transfer Dynamics in Two-Dimensional Nonmagnetic-Ferromagnetic van der Waals Heterostructures. <i>Nano Letters</i> , <b>2021</b> , 21, 3237-3244	11.5	9
26	A MoS2 and Graphene Alternately Stacking van der Waals Heterostructure for Li+/Mg2+ Co-Intercalation. <i>Advanced Functional Materials</i> , <b>2021</b> , 11, 2103214	15.6	9
25	Two-dimensional tetragonal GaOI and InOI sheets: In-plane anisotropic optical properties and application to photocatalytic water splitting. <i>Catalysis Today</i> , <b>2020</b> , 340, 178-182	5.3	8
24	Stable configurations and electronic structures of hydrogenated graphyne. <i>Computational Materials Science</i> , <b>2014</b> , 91, 274-278	3.2	7
23	Enhanced photocatalytic performance of CdO/g-C6N6 heterostructure. <i>Materials Research Express</i> , <b>2019</b> , 6, 035910	1.7	7
22	Tuning magnetism at the two-dimensional limit: a theoretical perspective. <i>Nanoscale</i> , <b>2021</b> , 13, 100000	7.7	6
21	Magnon-phonon interaction in antiferromagnetic two-dimensional MXenes. <i>Nanotechnology</i> , <b>2020</b> , 31, 435705	3.4	6
20	Intrinsic valley polarization in 2D magnetic MXenes: surface engineering induced spin-valley coupling. <i>Journal of Materials Chemistry C</i> , <b>2021</b> , 9, 11132-11141	7.1	6
19	Theoretical investigation of CO catalytic oxidation by a FePtSe2 monolayer. <i>RSC Advances</i> , <b>2017</b> , 7, 19639-19639	19.639	6
18	Palladium clusters on graphene support: An ab initio study. <i>Chemical Physics Letters</i> , <b>2016</b> , 646, 56-63	2.5	5
17	Magnetic control of single transition metal doped MoS2 through H/F chemical decoration. <i>Journal of Magnetism and Magnetic Materials</i> , <b>2017</b> , 422, 243-248	2.8	5
16	PdSSe: Two-dimensional pentagonal Janus structures with strong visible light absorption for photovoltaic and photocatalytic applications. <i>Vacuum</i> , <b>2020</b> , 181, 109649	3.7	5
15	Two unexplored two-dimensional MSe2 (M = Cd, Zn) structures as the photocatalysts of water splitting and the enhancement of their performances by strain. <i>Vacuum</i> , <b>2020</b> , 182, 109728	3.7	5
14	Regulating the electronic structure of ReS2 by Mo doping for electrocatalysis and lithium storage. <i>Chemical Engineering Journal</i> , <b>2021</b> , 414, 128811	14.7	5
13	Hydrogenation Induced Carrier Mobility Polarity Reversal in Monolayer AlN. <i>Physica Status Solidi - Rapid Research Letters</i> , <b>2017</b> , 11, 1700260	2.5	4
12	Origins of promising thermoelectric performance in quaternary selenide BaAg2SnSe4. <i>Applied Physics Express</i> , <b>2019</b> , 12, 071006	2.4	3
11	A novel class of one-dimensional TaTMTe (TM = Cr, Fe, Co and Ni) compounds with strain-switched magnetic states. <i>Physical Chemistry Chemical Physics</i> , <b>2018</b> , 20, 6990-6995	3.6	3

10	Exploring the stability and reactivity of Ni <sub>2</sub> P and Mo <sub>2</sub> C catalysts using ab initio atomistic thermodynamics and conceptual DFT approaches. <i>Biomass Conversion and Biorefinery</i> , <b>2017</b> , 7, 377-383	2.3	3
9	Robust Giant Magnetoresistance in 2D Van der Waals Molecular Magnetic Tunnel Junctions. <i>ACS Applied Materials &amp; Interfaces</i> , <b>2021</b> , 13, 36098-36105	9.5	3
8	Monolayer PC: A promising material for environmentally toxic nitrogen-containing multi gases. <i>Journal of Hazardous Materials</i> , <b>2022</b> , 422, 126761	12.8	3
7	Doping isolated one-dimensional antiferromagnetic semiconductor vanadium tetrasulfide (VS <sub>4</sub> ) nanowires with carriers induces half-metallicity. <i>Journal of Materials Chemistry C</i> , <b>2021</b> , 9, 3122-3128	7.1	2
6	Ultrafast Light-Induced Ferromagnetic State in Transition Metal Dichalcogenides Monolayers.. <i>Journal of Physical Chemistry Letters</i> , <b>2022</b> , 2765-2771	6.4	1
5	Tuning Magnetic Anisotropy in Two-Dimensional Metal-Semiconductor Janus van der Waals Heterostructures. <i>Journal of Physical Chemistry Letters</i> , <b>2021</b> , 12, 11308-11315	6.4	0
4	Interlayer-expanded MoS <sub>2</sub> containing structural water with enhanced Mg diffusion kinetics and durability. <i>ChemElectroChem</i> ,	4.3	0
3	Control of Polaronic Behavior and Carrier Lifetimes via Metal and Anion Alloying in Chalcogenide Perovskites. <i>Journal of Physical Chemistry Letters</i> , 4955-4962	6.4	0
2	Electronic structure and binding energy relaxation of ScZr atomic alloying. <i>Chemical Physics Letters</i> , <b>2016</b> , 657, 177-183	2.5	
1	CuTe <sub>2</sub> Cl Monolayer: An Unexplored 2D Hybrid Structure with the Coexistence of Remarkable Charge Separation and Visible Light Absorption. <i>Physica Status Solidi - Rapid Research Letters</i> , <b>2020</b> , 14, 1900554	2.5	