## Junjie He

## List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

63	1,633	22	39
papers	citations	h-index	g-index
67 ext. papers	2,116 ext. citations	<b>6.4</b> avg, IF	5.28 L-index

#	Paper	IF	Citations
63	Monolayer PC: A promising material for environmentally toxic nitrogen-containing multi gases. Journal of Hazardous Materials, <b>2022</b> , 422, 126761	12.8	3
62	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
61	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	O
60	Tuning magnetism at the two-dimensional limit: a theoretical perspective. Nanoscale, 2021,	7.7	6
59	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
58	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
57	Robust Giant Magnetoresistance in 2D Van der Waals Molecular Magnetic Tunnel Junctions. <i>ACS Applied Materials &amp; Discourse (Materials &amp; Discourse)</i> 13, 36098-36105	9.5	3
56	Doping isolated one-dimensional antiferromagnetic semiconductor vanadium tetrasulfide (VS4) nanowires with carriers induces half-metallicity. <i>Journal of Materials Chemistry C</i> , <b>2021</b> , 9, 3122-3128	7.1	2
55	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
54	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
53	Remarkably enhanced Curie temperature in monolayer CrI3 by hydrogen and oxygen adsorption: A first-principles calculations. <i>Computational Materials Science</i> , <b>2020</b> , 183, 109820	3.2	18
52	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
51	Band Gap Engineering in an Efficient Solar-Driven Interfacial Evaporation System. <i>ACS Applied Materials &amp; Materia</i>	9.5	23
50	CuTe2Cl 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	
49	Magnon-phonon interaction in antiferromagnetic two-dimensional MXenes. <i>Nanotechnology</i> , <b>2020</b> , 31, 435705	3.4	6
48	Optically Driven Ultrafast Magnetic Order Transitions in Two-Dimensional Ferrimagnetic MXenes. Journal of Physical Chemistry Letters, <b>2020</b> , 11, 6219-6226	6.4	15
47	Theoretical dissection of superconductivity in two-dimensional honeycomb borophene oxide B2O crystal with a high stability. <i>Npj Computational Materials</i> , <b>2020</b> , 6,	10.9	18

## (2018-2020)

46	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
45	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
44	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
43	Two-dimensional honeycomb borophene oxide: strong anisotropy and nodal loop transformation. <i>Nanoscale</i> , <b>2019</b> , 11, 2468-2475	7.7	62
42	Origins of promising thermoelectric performance in quaternary selenide BaAg2SnSe4. <i>Applied Physics Express</i> , <b>2019</b> , 12, 071006	2.4	3
41	Nitrogen-Doped MoS2 Foam for Fast Sodium Ion Storage. <i>Advanced Materials Interfaces</i> , <b>2019</b> , 6, 19004	<b>6</b> 06	28
40	Improving ionic/electronic conductivity of MoS2 Li-ion anode via manganese doping and structural optimization. <i>Chemical Engineering Journal</i> , <b>2019</b> , 372, 665-672	14.7	22
39	Remarkably enhanced ferromagnetism in a super-exchange governed Cr2Ge2Te6 monolayer via molecular adsorption. <i>Journal of Materials Chemistry C</i> , <b>2019</b> , 7, 5084-5093	7.1	32
38	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
37	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
36	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
35	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
34	Enhanced photocatalytic performance of CdO/g-C6N6 heterostructure. <i>Materials Research Express</i> , <b>2019</b> , 6, 035910	1.7	7
33	Synergistically Configuring Intrinsic Activity and Fin-Tube-Like Architecture of Mn-Doped MoS2-Based Catalyst for Improved Hydrogen Evolution Reaction. <i>ACS Applied Energy Materials</i> , <b>2019</b> , 2, 493-502	6.1	23
32	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
31	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
30	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
29	Low lattice thermal conductivity and promising thermoelectric figure of merit of Zintl type TlInTe2. Journal of Materials Chemistry C, <b>2018</b> , 6, 13269-13274	7.1	18

28	Two-dimensional MoS2-MoSe2 lateral superlattice with minimized lattice thermal conductivity. Journal of Applied Physics, <b>2018</b> , 124, 165101	2.5	15
27	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
26	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
25	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
24	Theoretical investigation of CO catalytic oxidation by a Fe <b>B</b> tSe2 monolayer. <i>RSC Advances</i> , <b>2017</b> , 7, 196	39. <del>-/</del> 196	538
23	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
22	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
21	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
20	Exploring the stability and reactivity of Ni2P and Mo2C 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
19	Anisotropic carrier mobility in buckled two-dimensional GaN. <i>Physical Chemistry Chemical Physics</i> , <b>2017</b> , 19, 23492-23496	3.6	14
18	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
17	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
16	Electronic structure and binding energy relaxation of ScZr atomic alloying. <i>Chemical Physics Letters</i> , <b>2016</b> , 657, 177-183	2.5	
15	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
14	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
13	Palladium clusters on graphene support: An ab initio study. <i>Chemical Physics Letters</i> , <b>2016</b> , 646, 56-63	2.5	5
12	Direct hydrodeoxygenation of phenol over carbon-supported Ru catalysts: A computational study. Journal of Molecular Catalysis A, <b>2016</b> , 423, 300-307		16
11	The surface stability and equilibrium crystal morphology of Ni2P nanoparticles and nanowires from an ab initio atomistic thermodynamic approach. <i>CrystEngComm</i> , <b>2016</b> , 18, 3808-3818	3.3	11

## LIST OF PUBLICATIONS

10	Prediction of half-semiconductor antiferromagnets with vanishing net magnetization. <i>RSC Advances</i> , <b>2015</b> , 5, 46640-46647	3.7	17
9	Strain control of the electronic structures, magnetic states, and magnetic anisotropy of Fe doped single-layer MoS2. <i>Computational Materials Science</i> , <b>2015</b> , 110, 102-108	3.2	41
8	Magnetic exchange coupling and anisotropy of 3d transition metal nanowires on graphyne. <i>Scientific Reports</i> , <b>2014</b> , 4, 4014	4.9	48
7	Spin Switch of the Transition-Metal-Doped Boron Nitride Sheet through H/F Chemical Decoration. Journal of Physical Chemistry C, <b>2014</b> , 118, 8899-8906	3.8	26
6	Stable configurations and electronic structures of hydrogenated graphyne. <i>Computational Materials Science</i> , <b>2014</b> , 91, 274-278	3.2	7
5	Indirect-direct band gap transition through electric tuning in bilayer MoS2. <i>Journal of Chemical Physics</i> , <b>2014</b> , 140, 174707	3.9	32
4	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
3	Interlayer Expanded MoS2 containing structural water with enhanced Mg Eiffusion kinetics and durability. Chem Electro Chem,	4.3	O
2	A MoS2 and Graphene Alternately Stacking van der Waals Heterostructure for Li+/Mg2+Co-Intercalation. <i>Advanced Functional Materials</i> ,2103214	15.6	9
1	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	O