

# Weiwei Sun

## List of Publications by Year in descending order

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39  
papers

1,585  
citations

394286

19  
h-index

315616

38  
g-index

39  
all docs

39  
docs citations

39  
times ranked

2597  
citing authors

#	ARTICLE	IF	CITATIONS
1	Direct Synthesis of Large-Area 2D Mo <sub>2</sub> C on In Situ Grown Graphene. <i>Advanced Materials</i> , 2017, 29, 1700072.	11.1	305
2	In situ atomistic insight into the growth mechanisms of single layer 2D transition metal carbides. <i>Nature Communications</i> , 2018, 9, 2266.	5.8	125
3	Computational Discovery and Design of MXenes for Energy Applications: Status, Successes, and Opportunities. <i>ACS Applied Materials &amp; Interfaces</i> , 2019, 11, 24885-24905.	4.0	105
4	Tracking ion intercalation into layered Ti <sub>3</sub> C <sub>2</sub> MXene films across length scales. <i>Energy and Environmental Science</i> , 2020, 13, 2549-2558.	15.6	100
5	Double transition metal MXenes with wide band gaps and novel magnetic properties. <i>Nanoscale</i> , 2018, 10, 11962-11968.	2.8	88
6	Effects of Surface Terminations of 2D Bi <sub>2</sub> WO <sub>6</sub> on Photocatalytic Hydrogen Evolution from Water Splitting. <i>ACS Applied Materials &amp; Interfaces</i> , 2020, 12, 20067-20074.	4.0	78
7	Low-Temperature Synthesis of Single Palladium Atoms Supported on Defective Hexagonal Boron Nitride Nanosheet for Chemoselective Hydrogenation of Cinnamaldehyde. <i>ACS Nano</i> , 2021, 15, 10175-10184.	7.3	77
8	Computational Screening of MXene Electrodes for Pseudocapacitive Energy Storage. <i>Journal of Physical Chemistry C</i> , 2019, 123, 315-321.	1.5	69
9	Edge Segregated Polymorphism in 2D Molybdenum Carbide. <i>Advanced Materials</i> , 2019, 31, e1808343.	11.1	56
10	Surface Reorganization Leads to Enhanced Photocatalytic Activity in Defective BiOCl. <i>Chemistry of Materials</i> , 2018, 30, 5128-5136.	3.2	55
11	Interfacial and electronic properties of heterostructures of MXene and graphene. <i>Physical Review B</i> , 2019, 99, .	1.1	53
12	Investigation of Charge-Transfer Interaction in Mixed Stack Donor-Acceptor Cocrystals Toward Tunable Solid-State Emission Characteristics. <i>Crystal Growth and Design</i> , 2018, 18, 6001-6008.	1.4	51
13	A new 2D monolayer BiXene, M <sub>2</sub> C (M = Mo, Tc, Os). <i>Nanoscale</i> , 2016, 8, 15753-15762.	2.8	46
14	Synergistic effects between polyvinylpyrrolidone and oxygen vacancies on improving the oxidase-mimetic activity of flower-like CeO <sub>2</sub> nanozymes. <i>Nanoscale</i> , 2020, 12, 19104-19111.	2.8	37
15	Understanding the electrochemical properties of A <sub>2</sub> MSiO <sub>4</sub> (A = Li and Na; M = Ti, Zr, Hf) calculations. <i>Journal of Materials Chemistry A</i> , 2016, 4, 17455-17463.	5.2	35
16	Multiscale and Multimodal Characterization of 2D Titanium Carbonitride MXene. <i>Advanced Materials Interfaces</i> , 2020, 7, 1902207.	1.9	35
17	Structure and energy of point defects in TiC: An <i>ab initio</i> study. <i>Physical Review B</i> , 2015, 91, .	1.1	23
18	High photon energy spectroscopy of NiO: Experiment and theory. <i>Physical Review B</i> , 2016, 93, .	1.1	22

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19	Dynamic stability of the single-layer transition metal dichalcogenides. Computational Materials Science, 2014, 92, 206-212.	1.4	19
20	Self-diffusion of Ti interstitial based point defects and complexes in TiC. Acta Materialia, 2019, 165, 381-387.	3.8	18
21	The role of group III, IV elements in Nb <sub>4</sub> AC <sub>3</sub> MAX phases (A = Al, Si, Ga, Ge) and the unusual anisotropic behavior of the electronic and optical properties. Physical Chemistry Chemical Physics, 2017, 19, 15471-15483.	1.3	17
22	Role of correlation and relativistic effects in MAX phases. Journal of Materials Science, 2012, 47, 7615-7620.	1.7	16
23	Investigations on electronic, Fermi surface, Curie temperature and optical properties of Zr <sub>2</sub> CoAl. Journal of Solid State Chemistry, 2017, 247, 97-104.	1.4	15
24	Stabilizing a hexagonal Ru <sub>2</sub> C via Lifshitz transition under pressure. Applied Physics Letters, 2013, 103, .	1.5	14
25	Anisotropic distortion and Lifshitz transition in $\text{Hf}_{1-x}\text{Zr}_x\text{C}$ under pressure. Physical Review B, 2017, 95, .	1.1	14
26	Solid emission color tuning of organic charge transfer cocrystals based on planar $\pi$ -conjugated donors and TCNB. Journal of Solid State Chemistry, 2019, 272, 96-101.	1.4	14
27	Strain and doping effects on the energetics of hydrogen desorption from the MgH <sub>2</sub> (001) surface. Europhysics Letters, 2013, 101, 27006.	0.7	13
28	Pushing the limit of thermal conductivity of MAX borides and MABs. Journal of Materials Science and Technology, 2022, 97, 79-88.	5.6	12
29	Combining configurational energies and forces for molecular force field optimization. Journal of Chemical Physics, 2017, 147, 161713.	1.2	11
30	A combined machine learning and density functional theory study of binary Ti-Nb and Ti-Zr alloys: Stability and Young's modulus. Computational Materials Science, 2020, 184, 109830.	1.4	10
31	Improvement in the desorption of H <sub>2</sub> from the MgH <sub>2</sub> (110) surface by means of doping and mechanical strain. Computational Materials Science, 2014, 86, 165-169.	1.4	9
32	Gluing together metallic and covalent layers to form Ru <sub>2</sub> C under ambient conditions. Physical Chemistry Chemical Physics, 2015, 17, 9730-9736.	1.3	9
33	Photoinduction of palladium single atoms supported on defect-containing $\text{Al}^{3+}$ -AlOOH nanoleaf for efficient trans-stilbene epoxidation. Chemical Engineering Journal, 2022, 429, 132149.	6.6	8
34	Stability of a new cubic monoxide of Thorium under pressure. Scientific Reports, 2015, 5, 13740.	1.6	7
35	The correlation between N deficiency and the mechanical properties of the Ti <sub>2</sub> AlN <sub>y</sub> MAX phase. Journal of the European Ceramic Society, 2020, 40, 2279-2286.	2.8	7
36	Li <sub>2</sub> FePO <sub>4</sub> F and its metal-doping for Li-ion batteries: an ab initio study. RSC Advances, 2014, 4, 50195-50201.	1.7	6

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37	Behavior of intrinsic defects in BaF <sub>2</sub> under uniaxial compressions: An ab initio investigation. <i>Materials Today Communications</i> , 2021, 28, 102730.	0.9	5
38	Observation of Square-Planar Distortion in Lanthanide-Doped Skutterudite Crystals. <i>Journal of Physical Chemistry C</i> , 2019, 123, 14632-14638.	1.5	1
39	Exchange of Re and Mo atoms in MoS <sub>2</sub> driven by Scanning Transmission Electron Microscopy. <i>Microscopy and Microanalysis</i> , 2017, 23, 1702-1703.	0.2	0