

# 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	Pushing the limit of thermal conductivity of MAX borides and MABs. <i>Journal of Materials Science and Technology</i> , 2022, 97, 79-88.	5.6	12
2	Photoinduction of palladium single atoms supported on defect-containing $\beta$ -AlOOH nanoleaf for efficient trans-stilbene epoxidation. <i>Chemical Engineering Journal</i> , 2022, 429, 132149.	6.6	8
3	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
4	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
5	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
6	A combined machine learning and density functional theory study of binary Ti-Nb and Ti-Zr alloys: Stability and Young's modulus. <i>Computational Materials Science</i> , 2020, 184, 109830.	1.4	10
7	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
8	The correlation between N deficiency and the mechanical properties of the Ti <sub>2</sub> AlN <sub>y</sub> MAX phase. <i>Journal of the European Ceramic Society</i> , 2020, 40, 2279-2286.	2.8	7
9	Multiscale and Multimodal Characterization of 2D Titanium Carbonitride MXene. <i>Advanced Materials Interfaces</i> , 2020, 7, 1902207.	1.9	35
10	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
11	Solid emission color tuning of organic charge transfer cocrystals based on planar $\pi$ -conjugated donors and TCNB. <i>Journal of Solid State Chemistry</i> , 2019, 272, 96-101.	1.4	14
12	Observation of Square-Planar Distortion in Lanthanide-Doped Skutterudite Crystals. <i>Journal of Physical Chemistry C</i> , 2019, 123, 14632-14638.	1.5	1
13	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
14	Edge Segregated Polymorphism in 2D Molybdenum Carbide. <i>Advanced Materials</i> , 2019, 31, e1808343.	11.1	56
15	Interfacial and electronic properties of heterostructures of MXene and graphene. <i>Physical Review B</i> , 2019, 99, .	1.1	53
16	Computational Screening of MXene Electrodes for Pseudocapacitive Energy Storage. <i>Journal of Physical Chemistry C</i> , 2019, 123, 315-321.	1.5	69
17	Self-diffusion of Ti interstitial based point defects and complexes in TiC. <i>Acta Materialia</i> , 2019, 165, 381-387.	3.8	18
18	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

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19	Surface Reorganization Leads to Enhanced Photocatalytic Activity in Defective BiOCl. Chemistry of Materials, 2018, 30, 5128-5136.	3.2	55
20	In situ atomistic insight into the growth mechanisms of single layer 2D transition metal carbides. Nature Communications, 2018, 9, 2266.	5.8	125
21	Double transition metal MXenes with wide band gaps and novel magnetic properties. Nanoscale, 2018, 10, 11962-11968.	2.8	88
22	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
23	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
24	Anisotropic distortion and Lifshitz transition in $\text{Hf}_{1-x}\text{Ta}_x$ under pressure. Physical Review B, 2017, 95, .	1.1	14
25	Direct Synthesis of Large Area 2D Mo <sub>2</sub> C on In Situ Grown Graphene. Advanced Materials, 2017, 29, 1700072.	11.1	305
26	Combining configurational energies and forces for molecular force field optimization. Journal of Chemical Physics, 2017, 147, 161713.	1.2	11
27	Exchange of Re and Mo atoms in MoS <sub>2</sub> driven by Scanning Transmission Electron Microscopy. Microscopy and Microanalysis, 2017, 23, 1702-1703.	0.2	0
28	A new 2D monolayer BiXene, M <sub>2</sub> C (M = Mo, Tc, Os). Nanoscale, 2016, 8, 15753-15762.	2.8	46
29	High photon energy spectroscopy of NiO: Experiment and theory. Physical Review B, 2016, 93, .	1.1	22
30	Understanding the electrochemical properties of A <sub>2</sub> MSiO <sub>4</sub> (A = Li and Na; M = Ti, Zr, Hf) by first-principles calculations. Journal of Materials Chemistry A, 2016, 4, 17455-17463.	5.2	35
31	Stability of a new cubic monoxide of Thorium under pressure. Scientific Reports, 2015, 5, 13740.	1.6	7
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	Structure and energy of point defects in TiC: An <i>ab initio</i> study. Physical Review B, 2015, 91, .	1.1	23
34	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
35	Li <sub>2</sub> FePO <sub>4</sub> F and its metal-doping for Li-ion batteries: an <i>ab initio</i> study. RSC Advances, 2014, 4, 50195-50201.	1.7	6
36	Dynamic stability of the single-layer transition metal dichalcogenides. Computational Materials Science, 2014, 92, 206-212.	1.4	19

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37	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
38	Stabilizing a hexagonal Ru <sub>2</sub> C via Lifshitz transition under pressure. Applied Physics Letters, 2013, 103, .	1.5	14
39	Role of correlation and relativistic effects in MAX phases. Journal of Materials Science, 2012, 47, 7615-7620.	1.7	16