## **Zhonglong Zhao**

## List of Publications by Citations

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#	Paper	IF	Citations
39	Pressure-induced metallization of dense (HB)HDwith high-Tc superconductivity. <i>Scientific Reports</i> , <b>2014</b> , 4, 6968	4.9	502
38	PdMo bimetallene for oxygen reduction catalysis. <i>Nature</i> , <b>2019</b> , 574, 81-85	50.4	456
37	Sub-6 nm Fully Ordered L10-PtNito Nanoparticles Enhance Oxygen Reduction via Co Doping Induced Ferromagnetism Enhancement and Optimized Surface Strain. <i>Advanced Energy Materials</i> , <b>2019</b> , 9, 1803771	21.8	76
36	CuN Nanocubes for Selective Electrochemical Reduction of CO to Ethylene. <i>Nano Letters</i> , <b>2019</b> , 19, 865	818663	3 76
35	Steering elementary steps towards efficient alkaline hydrogen evolution via size-dependent Ni/NiO nanoscale heterosurfaces. <i>National Science Review</i> , <b>2020</b> , 7, 27-36	10.8	71
34	Tungsten-Doped L1 -PtCo Ultrasmall Nanoparticles as a High-Performance Fuel Cell Cathode. <i>Angewandte Chemie - International Edition</i> , <b>2019</b> , 58, 15471-15477	16.4	62
33	Exclusive Strain Effect Boosts Overall Water Splitting in PdCu/Ir Core/Shell Nanocrystals. <i>Angewandte Chemie - International Edition</i> , <b>2021</b> , 60, 8243-8250	16.4	55
32	Biaxial Strains Mediated Oxygen Reduction Electrocatalysis on Fenton Reaction Resistant L10-PtZn Fuel Cell Cathode. <i>Advanced Energy Materials</i> , <b>2020</b> , 10, 2000179	21.8	54
31	Generalized Surface Coordination Number as an Activity Descriptor for CO2 Reduction on Cu Surfaces. <i>Journal of Physical Chemistry C</i> , <b>2016</b> , 120, 28125-28130	3.8	54
30	Computational Screening of Near-Surface Alloys for CO2 Electroreduction. ACS Catalysis, 2018, 8, 3885	-3:8,9:4	51
29	Nitrogen concentration driving the hardness of rhenium nitrides. Scientific Reports, 2014, 4, 4797	4.9	47
28	Lavender-Like Ga-Doped Pt3Co Nanowires for Highly Stable and Active Electrocatalysis. <i>ACS Catalysis</i> , <b>2020</b> , 10, 3018-3026	13.1	42
27	Cu-Based Single-Atom Catalysts Boost Electroreduction of CO2 to CH3OH: First-Principles Predictions. <i>Journal of Physical Chemistry C</i> , <b>2019</b> , 123, 4380-4387	3.8	40
26	Tuning the oxygen evolution reaction on a nickel-iron alloy via active straining. <i>Nanoscale</i> , <b>2019</b> , 11, 426	5- <del>4.3</del> 0	36
25	Sub-Monolayer YO /MoO on Ultrathin Pt Nanowires Boosts Alcohol Oxidation Electrocatalysis. <i>Advanced Materials</i> , <b>2021</b> , 33, e2103762	24	31
24	Modulated T carbon-like carbon allotropes: an ab initio study. RSC Advances, 2014, 4, 17364	3.7	28
23	Computational Discovery of Nickel-Based Catalysts for CO2 Reduction to Formic Acid. <i>Journal of Physical Chemistry C</i> , <b>2017</b> , 121, 20865-20870	3.8	27

## (2019-2015)

22	High pressure structures and superconductivity of AlH3(H2) predicted by first principles. <i>RSC Advances</i> , <b>2015</b> , 5, 5096-5101	3.7	26
21	Potentially superhard hcp CrN2 compound studied at high pressure. <i>Physical Review B</i> , <b>2016</b> , 93,	3.3	21
20	Phase diagram, mechanical properties, and electronic structure of Nb-N compounds under pressure. <i>Physical Chemistry Chemical Physics</i> , <b>2015</b> , 17, 22837-45	3.6	20
19	Miscibility and ordered structures of MgO-ZnO alloys under high pressure. <i>Scientific Reports</i> , <b>2014</b> , 4, 5759	4.9	19
18	The low coordination number of nitrogen in hard tungsten nitrides: a first-principles study. <i>Physical Chemistry Chemical Physics</i> , <b>2015</b> , 17, 13397-402	3.6	19
17	Improving the Stability of Non-Noble-Metal M-N-C Catalysts for Proton-Exchange-Membrane Fuel Cells through M-N Bond Length and Coordination Regulation. <i>Advanced Materials</i> , <b>2021</b> , 33, e2006613	24	19
16	First-principles study on the structural and electronic properties of metallic HfH2 under pressure. <i>Scientific Reports</i> , <b>2015</b> , 5, 11381	4.9	18
15	Tungsten-Doped L10-PtCo Ultrasmall Nanoparticles as a High-Performance Fuel Cell Cathode. <i>Angewandte Chemie</i> , <b>2019</b> , 131, 15617-15623	3.6	17
14	Effects of magnetic ordering and electron correlations on the stability of FeN. <i>RSC Advances</i> , <b>2015</b> , 5, 31270-31274	3.7	13
13	Ab initio study of germanium-hydride compounds under high pressure. <i>RSC Advances</i> , <b>2015</b> , 5, 19432-1	9438	12
12	A Novel High-Density Phase and Amorphization of Nitrogen-Rich 1H-Tetrazole (CHN) under High Pressure. <i>Scientific Reports</i> , <b>2017</b> , 7, 39249	4.9	10
11	Experimental verification of the high pressure crystal structures in NH3BH3. <i>Journal of Chemical Physics</i> , <b>2014</b> , 140, 244507	3.9	10
10	Bimetallenes for selective electrocatalytic conversion of CO2: a first-principles study. <i>Journal of Materials Chemistry A</i> , <b>2020</b> , 8, 12457-12462	13	6
9	Crystal structures and properties of the CH4H2 compound under high pressure. <i>RSC Advances</i> , <b>2014</b> , 4, 37569	3.7	6
8	Ab initio molecular dynamic study of solid-state transitions of ammonium nitrate. <i>Scientific Reports</i> , <b>2016</b> , 6, 18918	4.9	5
7	Pressure-Induced Amorphization and Recrystallization of SnI2. <i>Journal of Physical Chemistry C</i> , <b>2015</b> , 119, 19312-19317	3.8	4
6	High-pressure phase transition of MHI(M: Er, Ho). <i>Journal of Chemical Physics</i> , <b>2014</b> , 141, 054703	3.9	4
5	Highly Efficient AuPd Catalyst for Synthesizing Polybenzoxazole with Controlled Polymerization. <i>Matter</i> , <b>2019</b> , 1, 1631-1643	12.7	3

4 Crystal structures and properties of nitrogen oxides under high pressure. RSC Advances, 2015, 5, 10337331,03379

3	Oxygen Reduction: Biaxial Strains Mediated Oxygen Reduction Electrocatalysis on Fenton Reaction Resistant L10-PtZn Fuel Cell Cathode (Adv. Energy Mater. 29/2020). <i>Advanced Energy Materials</i> , <b>2020</b> , 10, 2070124	21.8	2
2	Pressure-induced structural changes in NH4Br. <i>Journal of Chemical Physics</i> , <b>2015</b> , 143, 064505	3.9	1
1	Circumventing the scaling relationship on bimetallic monolayer electrocatalysts for selective CO reduction <i>Chemical Science</i> , <b>2022</b> , 13, 3880-3887	9.4	1