

Assistant Professor Zhao Xunhua

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Academic Qualification:

Ph.D. in Physical Chemistry, Technische Universität Berlin, 2016

M.S. in Computational Chemistry, Graduate School of Chinese Academy of Sciences, 2011

B.A. in Chemical Engineering, Zhejiang University, 2007

Teaching Area

Molecular simulations, First-principles modeling for chemistry and materials sciences

Research Area

Modeling for Electrochemistry; Molecular Dynamics; Global Optimization; Machine Learning; Constant-potential MD;

2D materials; Interface Physics/Chemistry; Spectra Simulations

Working Experience

Assistant Professor, Macau University of Science and Technology, Macau, 2022-Present

Postdoc researchser, The University of Texas at Austin, 2018-2022

Postdoc researchser, Princeton University, 2016-2018

Selected Journal Papers

X. Bai*, X. Zhao*, Y. Zhang, C. Ling, Y. Zhou, J. Wang, Y. Liu, "Dynamic Stability of Copper Single-Atom Catalysts under Working Conditions", J. Am. Chem. Soc., Accepted, 2022. (*Equal contribution)

X. Li*, X. Zhao*, T. A. Hatton, Y. Liu, Y. Liu, "Redox-Tunable Lewis Bases for Electrochemical Carbon Dioxide Capture", Nat. Energy, Accepted, 2022. (*Equal contribution).

X. Zhao, Zachary H Levell, Saerom Yu, Y. Liu "Atomistic Understanding of Two-dimensional Electrocatalysts from First Principles", Chem. Rev., 122, 12, 10675, 2022. (Invited Review)

X. Zhao and Y. Liu "Origin of Selective Production of Hydrogen Peroxide by Electrochemical Oxygen Reduction", *J. Am. Chem. Soc.*, 143(25), 9423-9428, 2021.

X. Zhao and Y. Liu "Unveiling the Active Structure of Single Nickel Atom Catalysis: Critical Roles of Charge Capacity and Hydrogen Bonding", *J. Am. Chem. Soc.*, 142(12), 5773, 2020.