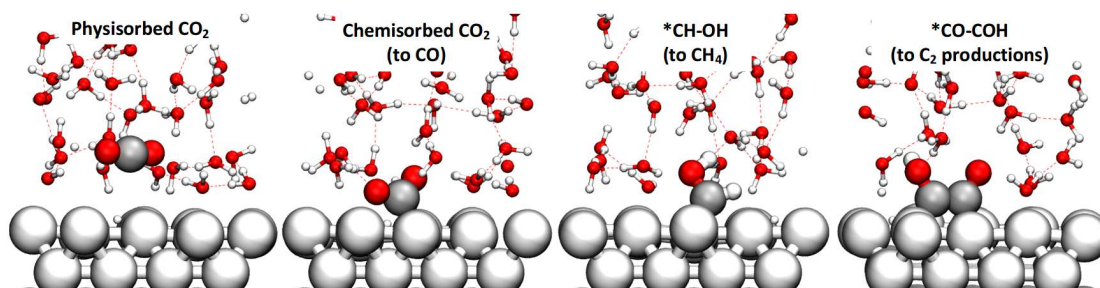


Multiscale Simulation of Carbon Dioxide Electro-Reaction

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Abstract: Carbon dioxide electro-reduction (CO₂ER) is a hot research topic of worldwide interest. To close the carbon loop, it is crucial to develop advanced "carbon utilization" technologies, among which CO₂ER is one the most promising techniques. Existing catalysts have low catalytic activity and poor selectivity and are not suitable for large-scale industrial applications. The development of high-performance catalysts requires a systematic and comprehensive understanding of the reaction mechanism of CO₂ER. Atomic-level-based multi-scale simulations provide a powerful tool to understand the CO₂ER microscopic mechanism. This presentation will report on the following four aspects: (a) Progress in the development of electrochemical theoretical methods,¹ with particular focus on the application of explicit solvent models² and constant voltage simulations³ to CO₂ER; (b) Development of CO₂ER reaction models and spectroscopic predictions; and (c) Progress in the application and theoretical studies of advanced nanomaterials⁴ and functional materials⁵ in CO₂ER. The insights from theoretical simulations pave a sound foundation for the rational design of catalytic materials. Theoretical simulations and experiments are mutually validated and complementary to each other, which is the general trend to accelerate materials development.



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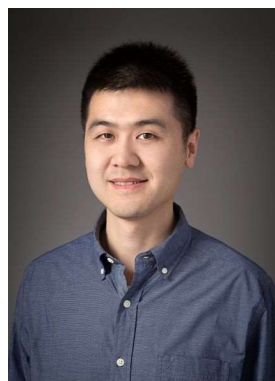
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Biography:



Dr. Tao Cheng received his Ph.D. degree from Shanghai Jiao Tong University in 2012 mentored by Prof. Huai Sun. He continued his research as a postdoctoral researcher at the California Institute of Technology (Caltech) from 2012 to 2015 with Prof. William A Goddard III. From 2015 to 2018, he worked as a research scientist at Joint Center for Artificial Photosynthesis at Caltech focusing on investigate the CO₂ reduction mechanism from simulation. He joined the Institute of Functional Nano and Soft Matter (FUNSOM) at Soochow University as a full professor in November 2018. His research focuses on applying the computational simulation method to solve problems in catalysis and energetic materials. He is particularly interested in the research of CO₂ electroreduction and solid electrolyte interfaces in lithium metal batteries. To date, he has published more than 90 peer-review journal papers with more than 3000 citations. Some of the papers have been published in *Science*, *Nat. Catal.*, *Nat. Chem.* His research has been selected as the cover illustration of *J. Am. Chem. Soc.* and has been highlighted and reviewed by *J. Am. Chem. Soc.* Spotlight and AIP. He has been invited, and served as a reviewer for more than 20 international journals.