

## Multi-Scale Modeling of Electrochemical CO<sub>2</sub>RR



21 January 2026

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Venue: N23-4018  
Time: 16:00 - 17:00  
Hosted by: Prof. Hui PAN

### Abstract

Electrochemical reduction reactions of carbon dioxide (eCO<sub>2</sub>RR) is an important way to realize carbon neutrality. However, the atomic understanding of eCO<sub>2</sub>RR mechanism at the interface between catalysts and electrolytes remains obscure. We combine constant-potential simulations and molecular dynamics modeling to systematically investigate the dynamic evolution of active sites and chemical space under reaction conditions, as well as their influence on eCO<sub>2</sub>RR performance. We unraveled the activity origin of eCO<sub>2</sub>RR to C<sub>2+</sub> products and clarified the importance of intermediate CO coverage on product selectivity. Besides, we also developed the coarse-grained modeling framework to explore the effect of mass transfer of electrolyte components on electrochemical performance.

### Biography

Prof. Yaqiong SU received his Master degree from Xiamen University in 2014 and PhD degree from Eindhoven University of Technology in 2018, and then did his postdoctoral research at Eindhoven University of Technology. He worked as a visiting scholar in 2011-iChEM, Xiamen University from January 2020 to August 2020. He is now a Distinguished Professor and Principal Investigator at School of Chemistry, Xi'an Jiaotong University. His research involves theoretical chemistry, computational catalysis and spectroscopic electrochemistry. He is the editorial board member of some journals, including Journal of Supercritical Fluids, ChemCatChem, Journal of Materials Informatics, AI for Materials, Current Catalysis, Photocatalysis: Researches and Potential. He has published 300 papers, including Science(2), PNAS(1), Nature Comm.(8), JACS(12), Angew. Chem.(20), Adv. Mater.(5), Energy Environ. Sci.(2), ACS Catal.(12), and so on.