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IAPME Seminar

Electroreduction Reaction Mechanism of Metal-nitrogen-carbon Catalysts through Numerical Simulations

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Venue: N23-3022
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Hosted by: Prof. Yongqing CAI

Abstract

With the rapid progress in computer science, numerical simulations, including density functional theory and molecular dynamics simulations become an important approach in physical science. With density functional theory calculations, we explored reaction mechanisms of electrochemical reactions, such as oxygen reduction and CO_2 reduction that play an important role in energy conversion and energy storage. Single-atom iron embedded in N-doped carbon (Fe-N-C) is among the most representative single-atomic catalysts (SACs) for electrochemical CO_2 reduction reaction (CO_2RR). Despite the simplicity of the active site, the CO_2-to-CO mechanism on Fe-N-C remains controversial. Firstly, there is a long debate regarding the rate-determining step (RDS) of the reactions. Secondly, recent computational and experimental studies are puzzled by the fact that the CO-poisoned Fe centers still remain highly active at high potentials. Thirdly, there are ongoing challenges in elucidating the high selectivity of hydrogen evolution reaction (HER) over CO_2RR at high potentials. In this work, we introduce a novel CO_2RR mechanism on Fe-N-C, which was inspired by the dynamic of active sites in biological systems. By employing grand-canonical density functional theory and kinetic Monte-Carlo, we found that the RDS is not fixed but changes with the applied potential. We demonstrated that our proposed dual-side mechanisms could clarify the reason behind the high catalytic activity of CO-poisoned metal centers, as well as the high selectivity of HER over CO_2RR at high potential. This study provides a fundamental explanation for long-standing puzzles of an important catalyst and calls for the importance of considering the dynamic of active sites in reaction mechanisms.

Biography

Prof. Shuzhou LI received his B.Sc, M.Sc, and PhD in chemistry from Nankai University, Peking University, and University of Wisconsin, respectively. After working as a postdoc in Northwestern University, he joined in Nanyang Technological University. Currently, he is a Professor in School of Materials Science and Engineering and his research interests are theoretical and computational material science. He has been focused on (1) Heterogeneous Catalysis; (2) Artificial Intelligence for Materials Discovery; (3) Flexible Electronics.