





Computationally exploring and discovering electrochemical CO2 reduction catalysts

Lecture of

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Electrochemistry has become a key player in establishing a global sustainable energy landscape. Unfortunately, most electrochemical processes are limited in their efficiency and selectivity which has prevented them to replace carbon-intensive industrial processes. Computational simulations can help on various sides to improve electrochemistry, from the fundamental, atomistic understanding, over multi-scale modeling of realistic devices up to high-throughput screening of electrocatalysts. In this talk, I want to summarize our group's efforts on these three points, with a particular focus on the electrochemical reduction of CO2.