Multicale modeling of electrochemical reduction of CO_2 using density functional theory and kinetic monte carlo simulation

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The electrochemical CO_2 reduction reaction (CO2 RR) using renewable electrical energy is a promising route for converting CO2 to useful chemicals. However, this reaction is complex and involves a number of species and reactions, mechanistic understanding of that reactions is required. Although many models with plausible reaction mechanism have been proposed, coverage effects of catalyst surface and mass transport effects are not considered in most models at the same time. Here, we develop a multi-scale model based on density functional theory (DFT) calculations, kinetic Monte Carlo (kMC) simulation and computational fluid dynamics (CFD) to describe trends in coverage effects and mass transport effects as well as reaction kinetics for electrochemical CO_2 RR over Ag catalysts. DFT data is mapped into kMC model for sequential calculations, and kMC and CFD simulation are iteratively performed.
Consequently, the impacts of adsorption energy, intermediate coverage and local pH can be thoroughly addressed by multi-scale analysis.