멀티스케일 모델링 접근법을 통한 전기화학촉매 시스템의 이해

임형규†, 신승재[1], 김형준[1]
강원대학교; [1]한국과학기술원
(hklim@kangwon.ac.kr†)

The electrified solid-liquid interface system is a core physicochemical component that existed in many types of electrochemical heterogeneous catalyst systems related to various energy and environmental applications, such as fuel-cell, lithium-ion battery, etc. Despite its widespread use in a variety of commercial applications, the detailed physicochemical understanding is still at an early stage due to the difficulty of analysis. From the recent rapid advances in computational hardware and software, the multi-scale simulation framework which utilizes both quantum and molecular mechanics modeling methods is a useful tool to analyze the complex electrified solid-liquid interface system in atomic/molecular-scales. In this presentation, I would present recent research results about understanding the electrified solid-liquid interface systems such as electrochemical CO_2 conversion and electrical double layer systems, etc. using own-developed multi-scale simulation frameworks, DFT-CES.