Multi-Scale Simulation Framework for Solid-Liquid Interface: Applications in Energy and Environmental Systems

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The solid-liquid interface is a core physico-chemical component existed in any heterogeneous reaction systems related with energy and environmental applications. Although it is widely used in various applications, the elucidation of physico-chemical properties in interface region is practically difficult. From the recent rapid advances in computational hardware and software, the first-principle quantum mechanics method and the molecular mechanics method are actively used in various research fields. Especially, the multi-scale simulation framework which utilizes both quantum and molecular mechanics methods is a useful tool to analyze the complex solid-liquid interface system. In this presentation, we have focused on the research results of various solid-liquid interface systems, such as CO_2 capture/conversion and electrical double layer capacitor etc., using general atomistic computer simulation methods and own-developed new multi-scale simulation method. I would like to introduce how the atomic-scale simulation approaches can interpret complex interfacial phenomena and provide valuable insights in various chemical engineering research fields.