Center for Molecular Spectroscopy and Dynamics, IBS-Korea University

IBS Center for Molecular Spectroscopy and Dynamics

Seminar

- **SPEAKER**
  Prof. Hyungjun Kim (Dep. of Chemistry, KAIST)

- **TITLE**
  Toward Understanding of Complex Solid-Liquid Interfaces

- **ABSTRACT**
  Chemistry at the interface of dissimilar materials and phases of matters is often very exotic compared to the bulk phase chemistry. In particular, solid-liquid interfaces have their own importance due to their ubiquity in a variety of applications, such as heterogeneous catalysts and electrochemical systems for sustainable energy conversion and storage. However, because of their high degree of complexity and difficulty in experimental characterizations, the molecular level of details at the solid-liquid interfaces are barely understood to date, which impedes the further development and optimization of the chemistry at the interface. In such case, theory can be the best and ideal option; however, there is no proper simulation method that can describe both phases at the full atomic level in a computationally efficient manner. We thus develop a first-principles based multiscale simulation method to understand, predict, and design the chemistry at the complex materials interface. In this talk, I will discuss our recently developed multiscale simulation method, coined as a density functional theory in classical explicit solvents (DFT-CES). Using DFT-CES, we demonstrate how theory and computational simulations can aid understanding the exotic chemistry at the solid-liquid interface, which can suggest a theoretical guideline for developing better materials interfaces, heterogeneous catalysts, and electrochemical systems.

- **DATE AND VENUE**
  May 29, 2019 (Wednesday, 5:00 - 6:00 pm)
  Seminar Room A (116), KU R&D Center

- **LANGUAGE**
  Korean

- **INVITED BY**
  Prof. Kyungwon Kwak