Center for Molecular Spectroscopy and Dynamics, IBS-Korea University

IBS Center for Molecular Spectroscopy and Dynamics

Seminar

- **SPEAKER**
  Prof. Eric Borguet (Dep. Of Chemistry, Temple University)

- **TITLE**
  Ultrabroadband vibrational spectroscopy and dynamics at aqueous interfaces

- **ABSTRACT**
  Interfacial water structure is key to many chemical and physical processes. It can be probed by vibrational sum-frequency generation (vSFG) spectroscopy as well as ultrafast time-resolved vSFG. The use of ultrabroadband IR pulses enable interfacial vibrational dephasing to be probed, revealing the presence of multiple OH species as well as their relative orientations – an alternative to heterodyne vSFG. However, a more complete microscopic understanding requires additional techniques such as molecular dynamics simulations. Our experiments show that in the absence of surface charge (pH 2), water at silica surfaces exhibits significantly slower OH stretch vibrational relaxation (~600 fs) compared to bulk water. However, at charged silica surfaces (e.g., pH 6), bulk-like fast dynamics (~200 fs) are observed at low ionic strength. This decelerates to ~600 fs with the addition of NaCl. In parallel, vSFG results demonstrated that silica interfacial water structure is most sensitive to ions at pH=6-8, correlating with the known salt and pH dependence of silica surface reactivity. Consequently, it is unclear whether the observed slowing of the vibrational dynamics is due to the reduction in the Debye length, or because of changes in the local hydrogen bonding environment caused by the electrolyte and how this might depend on the identity of the ions or the solid surface. Combining molecular dynamics simulations with spectroscopic and time-resolved vSFG experiments on aqueous Al2O3 interfaces, along with the use of a molecular probe SCN-, sheds light on the ongoing debate on the role of ions in interfacial water structure and whether the behavior of silica/water interfaces can be generalized to other aqueous interfaces.

- **DATE AND VENUE**
  September 16, 2019 (Monday, 5:00 - 6:00)
  Seminar Room B (119), KU R&D Center

- **INVITED BY**
  Director Minhaeng Cho

- **LANGUAGE**
  English