Center for Molecular Spectroscopy and Dynamics, IBS-Korea University

IBS Center for Molecular Spectroscopy and Dynamics

Seminar

- **SPEAKER**
  Dr. Youngseon Shim (Samsung Advanced of Institute of Technology)

- **TITLE**
  A theoretical and computational study of liquid dynamics

- **ABSTRACT**
  Highlights of our previous molecular dynamics (MD) simulation work on liquid systems, such as room-temperature ionic liquids and organic liquids, have been presented and briefly compared with experiments. Solvation structure and dynamics in a room-temperature ionic liquid were investigated via molecular dynamics computer simulations by employing a model diatomic solute. The effective polarity of the solvent, measured as solvation-induced stabilization of a dipolar solute, and solvent dynamic response, are consonant with a solvatochromic measurement. Dielectric relaxation, related polarization and conductivity of the ionic liquid, were also studied via molecular dynamics computer simulations. Two main bands of its dielectric loss spectrum, the absorption band in the microwave region and bi-modal far-IR band were analyzed. Roles played by ion reorientations and translations in governing dynamic and static dielectric properties of the ionic liquid are examined. A brief comparison with available experimental results was also made. As for electrochemical applications, electrolytes for carbon-based supercapacitors and Li-ion batteries, such as ionic liquids and mixed carbonates with Li salt, were studied. Electrolyte structure, ionic conductivity, and associated solvent dynamics were investigated via MD simulation.

- **DATE AND VENUE**
  February 12, 2019 (Tuesday, 5:00 - 6:00 pm)
  Seminar Room A (116), KU R&D Center

- **LANGUAGE**
  Korean

- **INVITED BY**

  Director Minhaeng Cho