Institute for Basic Science

IBS Center for Molecular Spectroscopy and Dynamics

COLLOQUIUM

■ SPEAKER

Prof. Kyung-Koo Lee (Department of Chemistry, Kunsan National University)

■ TITLE

Determination of the oxidation potentials of organic molecules: calculation and experiment

■ ABSTRACT

Electrolytes are a key component of electrochemical systems such as lithium-ion battery and supercapacitor. In order to effectively develop the novel electrolyte, computer simulation methods like quantum chemistry and molecular dynamics simulation can be used for a high-throughput virtual screening.
The oxidation potential, which is a crucial property of film-forming additives on cathode, can be determined by quantum calculation. In this talk, the procedure to appropriately estimate the oxidation potential of benzene derivative and thiophene derivative will be presented. By comparing the experimental solvation energy and calculated results with a series of cavity scaling factors, the optimal solvent cavity scaling factor of neutral molecules and radial radicals in propylene carbonate was determined. The procedure can allow one to predict the oxidation potential with an accuracy of below 100 mV.

■ DATE AND VENUE

September, 2016 (Friday, 5:00-6:00 p.m.)
Seminar room 116, R&D Center