Center for Molecular Spectroscopy and Dynamics, IBS-Korea University

IBS Center for Molecular Spectroscopy and Dynamics

Seminar

■ **SPEAKER**

Dr. Saptarsi Mondal (IBS Center for Molecular Spectroscopy and Dynamics)

■ **TITLE**

Role of Weak Noncovalent Interactions in the Solvation and Photophysical Properties of the Biologically and Atmospherically Relevant Molecules

■ **ABSTRACT**

Noncovalent interactions play an important role in several important biological and atmospheric processes. One of such important molecules is fluorinated molecules whose polar, hydrophobic and phase segregation property via weak fluorous interaction makes them useful in the different field of applications. However, our molecular level understanding about the hydrogen bond network, photophysical and solvation properties of the fluorinated molecules are sparse. The experimental and theoretical studies of fluorinated alcohols reveal that structural and hydrogen bond heterogeneity increases in fluorinated alcohols compared to ethanol (ETH) as fluorine acts as potential hydrogen bond acceptor apart from the hydroxyl group causing to decrease in average hydrogen bond strength of the bulk fluorinated alcohols than ETH. Unlike to the aqueous mixture of ETH, fluorination causes to switching of the hydrogen bonding of water molecules from the hydrophilic OH terminal to the hydrophobic fluorine terminal of alcohols resulting to the less clustering of water molecules and an increased hydrogen bond between water and fluorinated alcohols through cooperative effect.

Further, the photophysical and solvation properties of the probe and solvent containing fluorinated groups have been investigated using the upconversion and simulation methods to understand the role of fluorous interaction in these processes. The lifetime and solvation dynamics of coumarin 153 in 2,2,2-Trifluoroethanol observed to be slow compared to other systems which have been attributed to the fluorous interaction between the −CF3 group of the probe and the solvent. These results clearly describe that the substitution of fluorine not only changes the hydrogen bond network of the aqueous mixture of alcohol drastically but also affect the orientation and solvation properties of the probe molecules containing the fluorine groups. Finally, the effect of microhydration as well as photoelectron spectral properties of atmospherically important carbonyl sulfide (OCS) in its neutral and anionic form have been investigated to understand the role of noncovalent interaction of sulfur-containing molecules. The present study reveals that hydration increases the detachment energy of the OCS– by 3.2 eV using an analytical method which can be used to model the atmospheric reactions involving OCS in the absence of experimental data.

■ **DATE AND VENUE**
March 13, 2019 (Wednesday, 3:00 - 4:00 pm)
Seminar Room A (116), KU R&D Center

■ **LANGUAGE**
English