
COLLOQUIUM

■ **SPEAKER**

Dr. Kijeong Kwac (IBS Center for Molecular Spectroscopy and Dynamics)

■ **TITLE**

Structure and Dynamics of Hydrogen Bonds in Methanol-Acetonitrile Liquid Mixture and Confined Two-dimensional Water

■ **ABSTRACT**

Hydrogen bonds are ubiquitous and have major role in many situations involving biomolecules and materials interacting with water. In this seminar I present two topics in which hydrogen bonds are the main actor. The first part is about a molecular dynamics study on solvation dynamics of formylperylene dissolved in methanol-acetonitrile liquid mixture. I present results from equilibrium and non-equilibrium molecular dynamics simulations that relate the slowdown of the solvation dynamics to the formation of a hydrogen-bonded methanol oligomer, which is hydrogen-bonded to the carbonyl group of formylperylene. In the second part, the presentation is about molecular dynamics simulations to characterize the structure of water confined in between two MoS₂ sheets. Water spontaneously fills the region sandwiched by two MoS₂ sheets in ambient conditions to form a specific pattern in which a square ring structure is formed by four diamonds via H-bonds, while each diamond shares a corner in a perpendicular manner, yielding an intriguing isogonal tiling structure.

■ **DATE AND VENUE**

June 14, 2018 (Thursday, 1:00 - 2:00 pm)
Seminar Room 116, KU R&D Center

■ **LANGUAGE**

Korean