Center for Molecular Spectroscopy and Dynamics, IBS-Korea University

IBS Center for Molecular Spectroscopy and Dynamics

Seminar

■ **SPEAKER**
Dr. Jejoong Yoo (IBS Center for Self-assembly and Complexity)

■ **TITLE**
Challenges in molecular dynamics simulations of unfolded proteins and protein-DNA complexes

■ **ABSTRACT**
In the field of the molecular dynamics (MD) simulation based on physical chemistry, the problem of protein folding has been an important subject over decades. Currently, the state-of-the-art MD method can provide a fairly detailed view on the folding process in terms of several competing molecular interactions such as hydrogen bonds, charge–charge interactions, and hydrophobic collapses. However, as the field is moving toward new challenges such as intrinsically disordered peptides (IDPs) that function without a defined structure and the large-scale protein-DNA complexes, the force fields are revealing previously unknown problems. Importantly, it turned out that the force fields overestimate most attractive forces such as charge-charge interactions, cation-pi interactions, and hydrophobic collapses, promoting artificial aggregation of biomolecules in general. Here, we extend our years long effort to resolve the problems using our own unique method based on physical chemistry—the NBFIX approach. In this approach, the intermolecular forces are calibrated against colligative properties of model solutions such as osmotic pressure by making atom pair-specific adjustments to the non-bonded interactions. Using the simulations of folded and unfolded proteins, epigenetic control of DNA condensation, and the sliding DNA clamp, I will quantitatively evaluate the improvements made by our corrections. Overall, MD simulations utilizing our corrections show dramatically improved reproductions of experiments as well as successful predictions of previous unknown principles.

■ **DATE AND VENUE**
March 20, 2019 (Wednesday, 5:00 - 6:00 pm)
Seminar Room A (116), KU R&D Center

■ **LANGUAGE**
English

■ **INVITED BY**

Professor Kyungwon Kwak