# The First Understanding on Polydiacetylene Supramolecular Assemblies using Multi-scale Molecular Dynamic Simulation

최열교, 안동준†
고려대학교
(ahn@korea.ac.kr†)

π-Organics based on conjugated monomeric and polymeric systems are intriguing biomimetic materials for applications relating to chemical and biological sensors. These conjugated π-material systems have unique photoelectric properties that alter as exposed to specific viruses, toxins and chemicals. In recent years, computational chemistry has gained valuable theoretical insights and atomistic understandings in various research fields. Especially, coarse-grained molecular dynamic simulation achieved very successful high speed calculations in lipid bilayer assemblies. In this presentation, we present the first understanding using multi-scale molecular dynamic simulations on polydiacetylene supramolecular assemblies.