Reveal the structural mechanism of soft matter systems subject to different thermodynamic conditions and non-equilibrium processes using a complementary combination of neutron scattering and computational simulations

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The wide variety of soft matter structures subject to the changes of thermodynamics variables and non-equilibrium processes has led to many practical applications in various fields, such as biomedicine and energy materials fabrication. To control, design, and optimize new soft matter materials with tailored properties and functionalities, the fundamental physical picture behind their structural changes and stability is inevitably important. Generally, the molecular arrangement of soft matter constituents is determined by the balance between the intra-molecular and inter-particle interaction, thermal entropy effect, solute-solvent interaction, and externally applied fields. In this talk, I will introduce how to reveal the comprehensive structural information of some soft matter systems subject to different thermodynamic conditions and non-equilibrium processes. In the case of thermal equilibrium, I will talk about how to probe the self-assembly aggregation, geometric shape, and invasive water distributions of soft matter solution systems by using contrast variation neutron scattering. In the case of non-equilibrium processes, I will talk about how to extract the microscopic deformation and orientation of soft matter constituents using in-situ rheological neutron scattering measurements. The fundamental picture behind the structural parameters of soft matter will be briefly discussed. These results are either consistent with those predicted by documented computational simulations or verified by trajectory analysis of our computational simulations. They can provide a possible bridge between experimental measurements and computational theory to map out the fundamental particle interaction behind the structural changes and distortions under different environmental and external conditions.

Date : 2022/10/25 (Tue)
Place : S4-625
Time : 14:00-15:00

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