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Beyond Implicit Solvents: Advancing Soft Matter Simulations with Explicit Solvent Molecular Dynamics

Performing simulations of soft matter systems, particularly molecular dynamics simulations, often involves coarse-graining the system's description while preserving the particle nature of the model. This approach includes implicitly modeling the solvent as random forces acting on the particles, such as using a Langevin thermostat in an NVT ensemble simulation. This method reduces computation costs and speeds up the evolution of large-scale structures or features of the model due to the shallower energy barriers in the free energy landscape. However, in certain scenarios, explicitly modeling the solvent becomes necessary. For example, the inclusion of a polar solvent in the model allows for a more accurate representation of these systems at higher concentrations, where the assumptions of a continuum dielectric medium and screened hydrodynamics break down. It is also necessary to use explicit solvent in nonequilibrium molecular dynamics simulations for studies under mechanical deformation or an electric field. We present soft matter systems where the solvent was explicitly included in the model, including a polyelectrolyte in semi-dilute solutions under shear, and a lipid bilayer with a zwitterionic lipid head in a dipolar solvent with added salts and an applied oscillating electric field, causing a charge imbalance and enabling the membrane to act as a capacitor.

Topical Area

Soft matter: polymers, and complex fluids

Author: CARRILLO, Jan Michael (ORN L)

Presenter: CARRILLO, Jan Michael (ORN L)