Scientific Achievement

Computational molecular dynamics simulations were used to study three water-soluble polymers, PAM, PEO, and PNIPAAm, with combinations of three force-fields (FFs) and five water models; polymer and water FFs were shown to have considerable effects on sampling polymer conformations appropriately in solvated systems.

Significance and Impact

Water-soluble polymers, such as the three studied here, are useful in industrial and biomedical applications: this work serves to show that multiple properties need to be tested.

Research Details

A force field analysis was conducted by measuring the radius of gyration \(R_g\) of the polymer chains in water, solvent accessible surface area (SASA), radial distribution functions \(g(r)\) and relative shape anisotropy \(\kappa^2\).

- For PAM and PNIPAAm, three generalized force fields (DREIDING, GAFF and GAFF2) were tested in combination with five water models: SPC, SPC/E, TIP3P, TIP4P, and TIP4P/2005. In the case of PEO, the CHARMM C35r force field was applied and the c-TIP3P water model was evaluated in addition to the other water models.