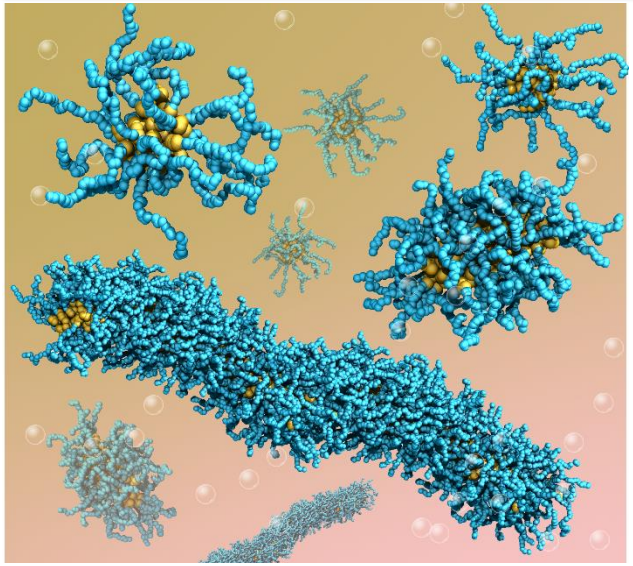
An Implicit Solvent Ionic Strength (ISIS) Method to Model Polyelectrolyte Systems with Dissipative Particle Dynamics

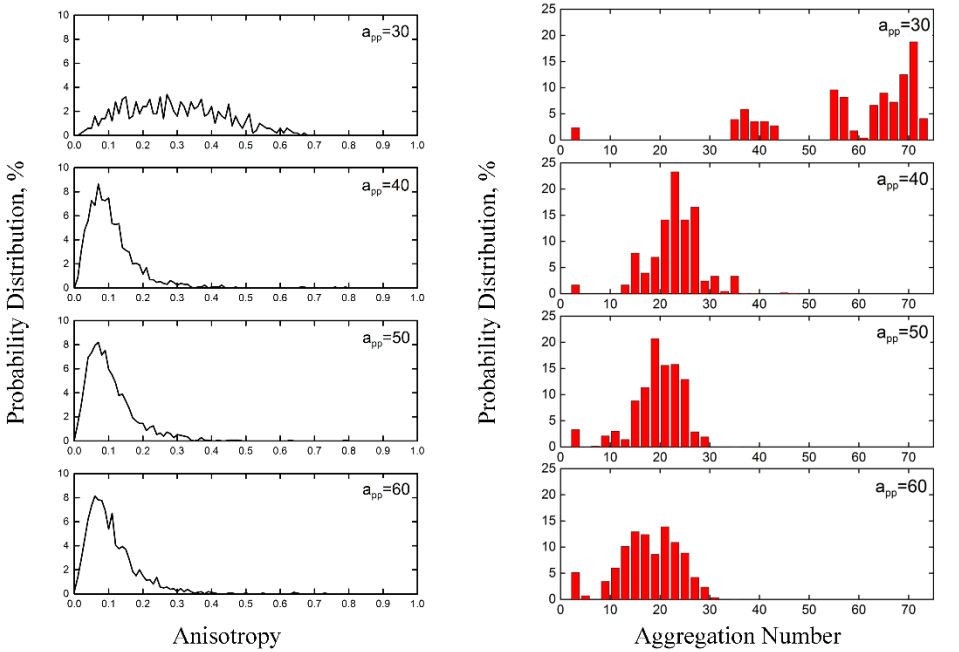


Researchers from North Carolina State University have developed a novel and versatile modeling strategy to simulate polyelectrolyte systems. The model has applications for creating new materials as well as for studying polyelectrolytes, including DNA and RNA.

Polyelectrolytes are chains of molecules that are positively or negatively charged when placed in water. Because they are sensitive to changes in their environment, polyelectrolytes hold promise for use in many industrial and biomedical applications.

Using the developed method the researchers can design novel polyelectrolyte-based materials and can effectively and efficiently investigate the salt dependence of conformational features of such materials in aqueous solutions.

The paper, "An implicit solvent ionic strength (ISIS) method to model polyelectrolyte systems with dissipative particle dynamics," is published online in the journal of Macromolecular Theory and Simulations.



Probability distribution of the anisotropy and the aggregation number of polyeletrolyte diblock micelles as a function of solvent ionic strength.