Structure and dynamics of polyelectrolyte

Polyelectrolytes (PEs) are polymers with charged repeating units which have ubiquitous applications, such as surfactants in personal care/health products, surface-modifiers in water treatment and oil recovery, additives in foods, superabsorbers in agriculture and sanitation, biomedical materials in implant coating and drug delivery, and electrolytes in lithium batteries. Biomacromolecules, like proteins, DNA and RNA, are also essentially PEs. Due to the competition between the short-range van der Waals interaction and the long-range electrostatic interaction, PEs exhibit complex structural, interfacial and dynamic behaviors. Theoretical modeling of PE systems remains an outstanding challenge. We developed a computational platform which combines the field theory and molecular simulation to investigate a variety of structural and dynamic properties of PEs. The theoretical approach systematically includes interactions with different effective ranges and self-consistently describe the coupling between the electrostatic interaction and the structural softness of polymers. With this is a powerful tool, we addressed several fundamental questions relevant to PEs, i.e. globule to pearl-necklace transition, finite size aggregates, absence of interfacial activity and “slow mode” in diffusion. This is also an ideal platform for exploring the potential applications of PEs in stimuli-responsive materials, energy storage and biomedical materials. Furthermore, the platform provides a fundamental step towards understanding challenges in biological systems, such as folding, binding, adsorption and translocation of proteins.

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