Brownian Dynamics Simulations on Hindered Diffusion of Single Polyelectrolyte Chain in Well-Defined Micro-Pores

최종훈, 전명석*
한국과학기술연구원
(mschun@kist.re.kr*)

The hindered diffusion is one of the crucial factors to understand the dynamic property of complex fluids in confined spaces. In comparison with the case of spherical colloids, the hindered diffusion of polyelectrolytes has more difficulty in both the theoretical investigations and the experiments, owing to many relevant parameters resulting from the complicated conformational properties of the polyelectrolyte chain. In this study, we performed the Brownian dynamics simulations upon a single polyelectrolyte confined in micro-pores where a coarse-grained bead-spring model incorporated with Debye-Hukel interaction would be adopted. For the given sizes of both the polyelectrolyte and the pore width, the hindered diffusion coefficient decreases as the solution ionic concentration decreases. Simulation results provide that the diffusive transport through the micro-pore is restricted by the influences of the steric hindrance of polyelectrolytes as well as the long-range electrostatic repulsion between the polyelectrolytes and the pore wall.