

Abstract Submitted
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Brownian Dynamics Simulations of Polyelectrolyte Adsorption in Shear Flow AJAY PANWAR, SATISH KUMAR, University of Minnesota — The adsorption of polyelectrolytes onto charged surfaces often occurs in microfluidic devices and can influence their operation. We employ Brownian dynamics simulations to investigate the effect of a simple shear flow on the adsorption of an isolated polyelectrolyte molecule onto an oppositely charged surface. The polyelectrolyte is modeled as a freely-jointed bead-rod chain where the total charge is distributed uniformly among all the beads, and the beads are allowed to interact with one another and the charged surface through screened Coulombic interactions. The simulations are performed by placing the chain some distance above the surface, and the adsorption behavior is studied as a function of the screening length. Specifically, we look at the components of the radius of gyration, normal and parallel to the adsorbing surface, as functions of the screening length, both in the absence and presence of the flow. We find that in the absence of flow, the chain lies flat and stretched on the adsorbing surface in the limit of weak screening, but attains free solution behavior in the limit of strong screening. In the presence of a shear flow, the chain orientation in the direction of the flow increases with increasing Weissenberg number over the entire range of screening lengths studied. We also find that increasing the strength of the shear flow leads to an increased contact of the chain with the surface compared to the case when no flow is present.

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