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Electric field driven motion of flexible polyelectrolytes in solution[1] TAK SHING LO, ANDREAS ACRIVOS, JOEL KOPLIK, Levich Institute, City College of CUNY, New York NY, BORIS KHUSID, Dept. of Mechanical Engineering, NJIT, Newark NJ — Our work aims to study dielectrophoresis of biomolecules in micro/nanofluidics, by combining electrohydrodynamics with molecular theories for the macromolecule polarization caused by the distortion of the counterion cloud. Molecular dynamics (MD) is used to simulate the transport of a flexible polyelectrolyte suspended in a solvent, with or without added salt, under the action of electric fields. We used a molecular model with explicit solvent atoms which includes automatically hydrodynamic interactions and finite atom size effects. The polyelectrolyte is modeled as a negatively charged freely-jointed bead-spring chain, and its responses in dc and ac fields are studied in detail. We focused on investigating the effects of the electric field on various physical quantities in comparison with equilibrium. We also developed a procedure to compute the dipole moments of the molecule and of the surrounding double layer, which are required for understanding the dielectrophoretic behavior of these molecules in nanoscopic channels.

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