Abstract Submitted
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Electric field driven motion of flexible polyelectrolytes[1] TAK SHING LO, Levich Institute, City College of CUNY, BORIS KHUSID, Dept. of Mechanical Engineering, NJIT, ANDREAS ACRIVOS, JOEL KOPLIK, Levich Institute, City College of CUNY — Our work aims to study dielectrophoresis of biomolecules in micro/nano-fluidics using molecular dynamics (MD) simulations. Our model combines electrohydrodynamics with molecular theories for the macromolecule polarization caused by the distortion of the counterion cloud. Unlike most available MD studies of polyelectrolytes, solvent atoms are explicitly represented in our model, so that hydrodynamic interactions are included naturally with no ad hoc assumption. The polyelectrolyte is modeled as a negatively charged bead-spring chain. The charges interact through the Coulomb potential and other molecular interactions are included via Lennard-Jones potentials. We study the transport properties of flexible polyelectrolytes suspended in a solvent, with or without added salt, under the action of DC or AC electric fields. MD data provide the information needed to compute the dipole moments of the molecule and the surrounding double layer, which are required for understanding the dielectrophoretic behavior of these molecules in nanoscopic channels.

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