

Abstract Submitted
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Counteracting the electrophoretic motion of a polyelectrolyte: a Molecular Dynamics study MARTIN M. BERTRAND, GARY W. SLATER, University of Ottawa — For a polyelectrolyte undergoing electrophoretic motion, it is predicted (D. Long, A. Ajdari, *Electrophoresis* 1996, 17:1161) that the mechanical force necessary to counteract the electrical force exerted on the molecule should be substantially smaller than the latter. In our work we examine this prediction using coarse grained Molecular Dynamics simulations in which we explicitly include the polymer, the solvent, the counterions and added salt. We measure the mechanical force required to counteract the electrophoretic motion and observe and quantify the resulting polymer conformations. One end of the polyelectrolyte is tethered to a fixed point in space via a harmonic potential. We measure the average counteracting force by monitoring the distance between the fixed point and the end of the molecule. Our simulations are carried out in a long cylindrical capillary with periodic boundary conditions.

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