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Polyelectrolytes in electric fields: An explicit solvent simulation study HONGJUN LIU, EDWARD MAGINN, Y. ELAINE ZHU, University of Notre Dame, Department of Chemical and Biomolecular Engineering — We use a coarse-grained molecular dynamics model to study the electrophoretic behavior of a flexible polyelectrolyte chain in a salt-free solution. The explicit solvent is used to recover the hydrodynamic interaction. Our results show the an excellence correspondence of simulation to experimental observations when the hydrodynamic interaction is considered. Electrophoretic mobility increases with the increasing chain length, passes through a maximum and reaches a plateau for the long polymers. Effective charge and effective friction are also investigated to provide the physical insight.

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