Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Stretching a strong polyelectrolyte chain under AC-electric fields: A molecular dynamics 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 method to study the structural dynamics of a single strong polyelectrolyte in an explicit salt solution under AC-electric fields. The conformational dimension of the polyelectrolyte chain in aqueous solutions added with trivalent counterions is investigated as a function of AC-electric field strength and frequency. Our simulation results show that the polyelectrolyte chain can be stretched when the applied AC-field strength exceeds a critical value at the AC frequency range comparable to or smaller than the reciprocal of the relaxation time of the polyelectrolyte chain. We also observe the curious breathing mode of the stretched polyelectrolyte with the applied AC-electric oscillation, which could be applied to effectively manipulate and assemble charged polymers and biopolymers with desirable structures by varied electric fields.

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Date submitted: 01 Dec 2009 Electronic form version 1.4