Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Mesoscopic Simulations of Free Solution Electrophoresis of Polyelectrolytes with Finite Debye Length GARY SLATER, OWEN HICKEY, TYLER SHENDRUK, University of Ottawa — The mobility of charged oligomers results from a complex interplay between electrostatic and hydrodynamic interactions leading to a competition between counter-ion condensation and cooperative shearing within the diffuse layer. Simulations of polyelectrolytes that include explicit ions are computationally expensive, while algorithms that couple infinitely thin Debye layers to mesoscopic fluid models are only useful in the long chain limit because they fail to predict the rise and non-monotonicity of the mobility. We present a hybrid mesoscale simulation technique that utilizes multi-particle collision dynamics (MPCD) to simulate surrounding solvent molecules and the Debye-Hückel approximation to assign effective charge to the MPCD particles. This hybrid scheme can capture the electro-hydrodynamics without having to explicitly include counter-ions or make costly electrostatic calculations. This MPCD-MD Debye-Hückel method shows great potential for simulating electrophoretic behavior of polyelectrolytes in novel microfluidic devices.

Tyler Shendruk
University of Ottawa

Date submitted: 10 Nov 2011 Electronic form version 1.4