Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Viscosity and scattering function of dilute, semidilute and concentrated polyelectrolyte solution: Molecular dynamics simulations[1] QI LIAO, Institute of Chemistry, the Chinese Academy of Sciences — We present the results of viscosity and scattering function of polyelectrolyte solutions in different solvent conditions for polymer backbone by molecular dynamics simulations. Polyelectrolyte solutions are modeled as an ensemble of bead-spring chains of charged Lennard-Jones particles with explicit counterions. Simulations were performed for both fully and partially charged polyelectrolyte chains with the number of monomers in the range of polymer concentrations covering both dilute and semidilute regime, even to the concentrated regime. The crossover behaviors of different regimes observed in the experiments are repeated quantitatively in our simulations.

[1]Acknowledgements: This work is financially supported by NSFC Grant Nos. 20974115 and 20674091.

Qi Liao
Institute of Chemistry, the Chinese Academy of Sciences

Date submitted: 17 Nov 2009 Electronic form version 1.4