

Abstract Submitted  
for the MAR14 Meeting of  
The American Physical Society

**Atomistic molecular dynamics simulations of the structure of symmetric Polyelectrolyte block copolymer micelle in salt-free aqueous solution**<sup>1</sup> RAJALAKSHMI CHOCKALINGAM, UPENDRA NATARAJAN, Indian Inst of Tech-Madras — The structure of a symmetric polystyrene-*b*-poly(acrylic acid) (PS-*b*-PAA) micelle in salt-free aqueous solution as a function of degree-of-neutralization (or ionization,  $f$ ) of the PAA is studied via explicit-atom-ion MD simulations, for the first time for a polyelectrolyte block copolymer in a polar solvent. Micelle size increases with  $f$  in agreement with experimental observations in literature, due to extension of PAA at higher ionization. Pair RDF's with respect to water oxygens show that corona-water interaction becomes stronger with  $f$  due to an increase in number density of carboxylate ( $\text{COO}^-$ ) groups on the chain. Water-PAA coordination (carboxylate O's) increases with ionization. H-bonding between PAA and water increases with  $f$  due to greater extent of corona-water affinity. With increase in  $f$ , atom and counter-ion  $\rho$  profiles confirm extension of corona blocks and micelle existing in the "osmotic regime," and a decrease in scattering peak intensity, in agreement with neutron scattering experiments and mean-field theory in literature. Inter-chain distance in PS core is found to decrease with ionization.

<sup>1</sup>Macromolecular Simulation and Modeling Laboratory, Dept. of Chemical Engineering, Indian Institute of Technology Madras, Chennai 600036.

Rajalakshmi Chockalingam  
Indian Inst of Tech-Madras

Date submitted: 04 Nov 2013

Electronic form version 1.4