

MAR14-2013-020330

Abstract for an Invited Paper  
for the MAR14 Meeting of  
the American Physical Society

### **Where Scattering and Computations Meet: Structure and Dynamics of Ionic Co-Polymers<sup>1</sup>**

DVORA PERAHIA, Clemson University

Ion transporting polymers constitute vital components in clean energy generation and storage devices including electrolytic media in fuel cells and ion conducting separators in batteries. While different polymers are currently in use, achieving controlled ion transport and storage ability while retaining mechanical and chemical stability remains a challenge: under the conditions which optimize the transport and storage for specific application, either mechanical or chemical stabilities are compromised. Designing block-co-polymers with ion transporting blocks bound to blocks that enhance mechanical and chemical stability would mitigate the challenge. Tailoring block copolymers with blocks that exhibit various desired properties, results in a new set of open questions that pertain to new complex materials including defining the phase diagram and understanding the interfacial regions of the multiblocks. Here we present the first molecular-level computational insight of the behavior of a pentablock, A-B-C-B-A, co-polymer that consists of an A block of poly(*t*-butyl-styrene), a B block of ethylene-*r*-propylene and a C block of a randomly sulfonated styrene, in solution in comparison with neutron scattering data. Neutron studies have shown that in hydrophobic solvents this pentablock forms elongated micelles in dilute solutions where the ionic block dominates the solution structure. These studies provide ensemble average of structure and properties. The computational studies provided further molecular-level insight. Here we will discuss the interrelations between scattering results and computational studies to provide remarkable understanding of a complex ionic system. Pathways to advance this molecular understanding to an actual membrane will be then discussed.

<sup>1</sup>We thank DOE contact DE-FGO2-12ER46843 for support of this work.