

Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

From a single molecule to a membrane of structured ionic polymers: A molecular dynamic simulation study DIPAK ARYAL, DVORA PERAHIA, Clemson University, GARY S. GREEST, Sandia National Laboratories — The association of an A-B-C-B-A co-polymer with an ionizable center and a bulky end block has been investigated using molecular dynamic simulations. The center block consists of a randomly sulfonated polystyrene connected to a flexible poly (ethylene-r-propylene) bridge and end capped with poly (t-butyl styrene). Tailoring the nature of individual segments within a block co-polymer is a potential design tool to form membranes with desired properties. The association mode and the dynamics of the segments control the overall characteristics. The membranes with three sulfonation level for the center block were made by evaporating a common solvent for all blocks. The local structure including size and distribution of the ionic blocks and the continuity of the styrene phase as well as long range correlations were identified at 300 and 500K. The initial membrane structure is affected by the structure in solution. Studies on changes that take place above the glass transition temperature for each of the blocks will also be presented.

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Date submitted: 15 Nov 2011

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