

Abstract Submitted
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Molecular Dynamics Simulations of a Single Chain Pentablock Ionomer in Dilute Solutions¹ DIPAK ARYAL, DVORA PERAHIA, Clemson University, GARY S. GREEST, Sandia National Laboratories — Co-polymers are in the core of many applications such as fuel cells, batteries and purification membranes that require transport across membranes. The challenge remains however that under the condition that transport is optimized, the stability of the membranes is compromised. To surmount this challenge, co-polymers with blocks targeting specific roles have been designed. Using molecular dynamics simulations we have studied the structure and dynamics of ionic single chain pentablock copolymer (*A-B-C-B-A*) containing randomly sulfonated polystyrene in the center, tethered to poly-ethylene-r-propylene end-capped by poly-*t*-butyl styrene. The ionic block facilitates transport while the A and B component are incorporated for mechanical stability. The conformation and dynamics of single pentablock ionomer of molecular weight $M_w = 50,000\text{g/mol}$ in an implicit poor solvent with dielectric constant of 1 and 77.7, water, and mixture (1:1) of cyclohexane and n-heptane at 300K and 500K will be presented. The effect of solvents on conformation of a single molecule of pentablock was determined and compared with experiment, providing a stepping stone to the understanding phase behavior of this polymer.

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