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Association of Multi-Chain Pentablock Ionomers in Solutions: A Molecular Dynamics Simulation Study[1] DIPAK ARYAL, DVORA PERAHIA, THUSITHA ETAMPAWALA, Clemson University, Clemson,SC,29634, GARY GREST, Sandia National Laboratories, Albuquerque, NM — Ionic block copolymers in solutions are of interest due to their fascinating ability to self-assemble into a variety of ordered microscopic structures such as ionic domains and hydrocarbon domains. These polymers show unique properties such as chemical and mechanical stability that arise from incompatibility between individual blocks, proton conductivity, ion transportability, and hydrophilicity. Using molecular dynamics simulations we have studied the association of multi-chain pentablock copolymers (A-B-C-B-A) in a 1:1 mixture of cyclohexane and heptane (mutual solvent), and in water at 300K and 500K. The center block consists of randomly sulfonated polystyrene connected to a flexible poly (ethylene-r-propylene) bridge and end caped with poly (t-butyl styrene). We found that the pentablock in mutual solvent forms micelles in solutions with the sulfonated polystyrene in the core and chains of swollen flexible poly (ethylene-r-propylene) and poly (t-butyl styrene) in the corona. In water, the micelle remains quasi-spherical with the ionic groups located on the outer surface at both temperatures. These results are good agreement with those obtained from small angle neutron scattering (SANS).

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