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Nano Aggregation of Structured Ionic Copolymers: Molecular Dynamics Simulation Study[1] DIPAK ARYAL, DVORA PERAHIA, Clemson University, GARY S. GREST, Sandia National Laboratories — Driven by mutual segregation, block copolymers exhibit a fascinating ability to self-assemble into a variety of ordered mesoscopic structures. Incorporating an ionizable block enhances incompatibility that together with tailoring blocks for specific functions presents an immense step towards engineering controlled transport systems. Here the interplay between the interactions of solvents with the specific blocks of a pentablock with a randomly sulfonated polystyrene center, tailored for transport, tethered to flexible poly (ethylene-r-propylene) end-capped with poly (t-butyl styrene) is studied by fully atomistic molecular dynamics simulations. The assembly of 2 to 30 macromolecules, in water results in a spherical tightly packed aggregate in which the ionizable blocks dominates the water interface. Transferred to a cyclohexane-heptane mixture, the hydrophobic blocks migrate to the interface. Surprisingly however, the ionic blocks form a nano-network rather than a corona. Further, this network also develops when assembled from hydrophobic solvents, where now the hydrophobic blocks dominate the interface. This network only slightly contracts or expands as the solvent is changed while concurrently the hydrophobic blocks migrate towards or a way from the solvent interface.

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