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Computational Insight into Solvent Effects on Conformation and Assembly of Structured Ionic Polymer[1] MANJULA SENANAYAKE, DIPAK ARYAL, DVORA PERAHIA, Clemson University, GARY GREST, Sandia National Laboratories — Structured ionomers are in the core of numerous current and potential new applications including clean energy, water purification membranes and sensors. The ability to facilitate ions and solvents transport is a key to their function and is controlled by their structure. One effective path for structural control is tuning their conformation by solvent interactions. Here, the confirmation and association of an ABCBA co-polymer where C is a randomly sulfonated polystyrene with sulfonation fractions $f = 0$ to 0.55, B is poly (ethylene-r-propylene), and A is poly (t-butyl styrene), in n-propanol are studied by molecular dynamic simulation. In contrast to the collapsed conformation of the ionizable block in hydrophobic solvents, we find that it remains swollen. Similar to hydrophobic solutions the co-polymers aggregate to form an ionizable core surrounded by extended hydrophobic chains. In contrast to the "locked-in" ionizable segments observed in cyclohexane/heptane, here the ionic clusters remain dynamic.

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