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Coarse graining of polystyrene sulfonate[1] DVORA PERAHIA, ANUPRIYA AGRAWAL, Clemson University, GARY S. GREST, Sandia National Laboratories — Capturing large length scales in soft matter while retaining atomistic properties is imperative to computational studies. Here we develop a new coarse-grained model for polystyrene sulfonate (PSS) that often serves as a model system because of its narrow molecular weight distribution and defined degree of sulfonation. Four beads are used to represent polymer where the backbone, the phenyl group, and the sulfonated group are each represented by a different bead and the fourth one represents counterion, which is sodium in our case. Initial atomistic simulations of PSS melt with sulfonation levels of 2-10%, with a dielectric constant ε =1 revealed a "locked" phase where motion of the polymer is limited. Dielectric constant of ε =5 was used to accelerate the dynamics. Bonded interactions were obtained using Boltzmann inversion on the bonded distributions extracted from atomistic simulation. Non-bonded interaction of polystyrene monomer was taken from our previous work and potential of mean force was used as the initial guess for interaction of the ionic beads. This set of potential was subsequently iterated to get a good match with radial distribution functions. This potential and its transferability across dielectric constants and temperatures will be presented.

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