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Structure and Dynamics Ionic Block co-Polymer Melts: Computational Study[1] DIPAK ARYAL, DVORA PERAHIA, Clemson University, GARY S. GREST, Sandia National Laboratories — Tethering ionomer blocks into co-polymers enables engineering of polymeric systems designed to encompass transport while controlling structure. Here the structure and dynamics of symmetric pentablock copolymers melts are probed by fully atomistic molecular dynamics simulations. The center block consists of randomly sulfonated polystyrene with sulfonation fractions f = 0 to 0.55 tethered to a hydrogenated polyisoprene (PI), end caped with poly(t-butyl styrene). We find that melts with f =0.15 and 0.30 consist of isolated ionic clusters whereas melts with f = 0.55 exhibit a long-range percolating ionic network. Similar to polystyrene sulfonate, a small number of ionic clusters slow the mobility of the center of mass of the co-polymer, however, formation of the ionic clusters is slower and they are often intertwined with PI segments. Surprisingly, the segmental dynamics of the other blocks are also affected.

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