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Computer Simulations of Aggregate Formation and Dynamics in Ionomers MONOJOY GOSWAMI[1], Rensselaer Polytechnic Institute, SANAT KUMAR, Rensselaer Polytechnic Institute, GERASSIMOS ORKOULAS, University of California, Los Angeles, ANIKET BHATTACHARYA, University of Central Florida — We investigate the structure and the dynamics of aggregate formation in ionomers, through the device of Monte Carlo (MC) and Brownian Dynamics (BD) simulations in the canonical ensemble. We carried out several computer experiments for different temperatures, different chain length and also for different charge states of counterions. Our result shows the formation of aggregates in telechelic ionomers. Pair distribution function for counterions clearly shows cluster formation at low temperatures. At high temperature, for longer chain lengths BD shows clear spherical structure which qualitatively matches with the experimental findings. For longer chain lengths, vesicular structure has been seen which is consistent with experimental findings.

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