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Molecular Dynamics Simulation of Ion Solvation in Polymer Melts: Effects of Dielectric Inhomogeneity and Chain Connectivity on Solvation Energy of Ions[1] LIJUN LIU[2], ISSEI NAKAMURA, State Key Laboratory of Polymer Physics and Chemistry, Changchun Institute of Applied Chemistry, Chinese Academy of Sciences — We study the ion solvation in block copolymer melts and polymer blends using molecular dynamics simulations. In our simulations, polymers are formed through the connection of beads that provide the dielectric response. Thus, we highlight the effect of the dielectric contrast between different species on the solvation energy of ions. We demonstrate the local enrichment of higher-dielectric components near ions, which corresponds well with the result of mean-field theories. Moreover, the chain connectivity significantly affects the reorientation of molecular dipoles in response to the electrostatic field from ions. Thus, we illustrate the marked difference in the solvation energy between the block copolymer and polymer blend. Importantly, the solvation energy substantially depends on the chain length of the polymers, in stark contrast to the Born solvation energy. We also show that our simulation results exhibit striking similarity to the result of the recent self-consistent mean field theories. However, for strongly correlated dipoles and ions, our simulations provide qualitatively opposite behaviors to these results, suggesting further development of the theoretical frameworks.

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[2]I use my CPS ID in this submission.

State Key Laboratory of Polymer Physics and Chemistry, Changchun Institute of Applied Chemistry, Chinese A

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