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Molecular Dynamics Simulations of Ion-Doped Microphase Separated Diblock Copolymers[1] YOUNGMI SEO, JONATHAN R. BROWN, LISA M. HALL, Ohio State Univ - Columbus — The effects of ion doping on microphase separated block copolymers are crucial to understand for transport applications such as battery electrolytes or fuel cell membranes. Prior experiments and theories have observed interesting trends, e.g. ions generally increase effective χ, broaden the domain interface at high loadings, and significantly change the order-to-disorder transition point. To provide a molecular level understanding of these trends and further information about ion dynamics, in this study, we perform molecular dynamics (MD) simulations using a generic coarse-grained model. We capture the selective ion solvation in one polymer microphase by adding an $1/r^4$ term to the intermolecular potential to account for the charge induced dipole effect between cations and A monomers. The model was validated by comparing with experimental domain spacing and density profile results. We find that as ions are added, the lamellar interface becomes sharper at first, then broadens with further ion loading, and finally forms a cylindrical morphology. We also observe that the interfacial broadening is retarded as the associative interaction between cations and A monomers or the ion-ion interaction strength is increased. These observations are compared to the results from fluids density functional theory (fDFT) which uses a similar model. We analyze ion dynamics in the model systems and discuss the impacts of ion selectivity and other variables on transport.

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Youngmi Seo
Ohio State Univ - Columbus

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