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Ionic Groups Enhanced Microphase Separation of Diblock Copolymers[1] JING ZONG, DONG MENG, Mississippi State Univ — Placement of ionic functionality on block copolymers, if properly designed, is known to generate more uniform nanoclusters and enhanced microphase separation. While recent experiments have demonstrated the effectiveness of this strategy, understanding from a computational point of view would reveal insightful information for systematic development and optimization of the approach. Here we apply our newly developed particle-field hybrid simulation formalism to study the microphase separation of a symmetric diblock copolymer (DBC) with the two blocks connected by an ionic junction group. In our simulations electrostatic interactions are taken into account explicitly, while the mean-field approximation is invoked for Flory-Huggins interactions. The method offers advantages in efficiently resolving both mesoscale self-assembled structures and structures due to strong correlations of electrostatic interactions. We show that inclusion of a single ionic group at the junction is able to drive DBC from the disordered into ordered state, agreeing with experimental observations [1]. Segregation is further enhanced by inclusion of multivalence ions as the result of the "bridging effect". Distribution of ions, while concentrated within the lamellar interfacial domains, also exhibit highly ordered in-plane structures. For multivalence case, charge neutrality analysis suggests existence of alternating positively-negatively charged layers in direction normal to lamellar interfaces. [1] ACS Macro Lett. 2015, 4, 1332-1336

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