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Local dielectric constant and its effects on the microphase separation in charged-neutral diblock copolymer melts RAJEEV KUMAR, National Center for Computational Sciences, Oak Ridge National Lab, Oak Ridge, TN- 37831, SCOTT SIDES, Tech-X Corporation, Boulder, CO - 80303, BOBBY SUMPTER, Computer Science and Mathematics Division & Center for Nanophase Materials Sciences, Oak Ridge National Lab, Oak Ridge, TN- 37831 — Using block copolymers as mesoscale templates has potential applications for improved photovoltaic devices and fuel-cells. Charged species in these polyelectrolytic copolymers play a vital role in determining the details of the nanoscale morphologies formed when these systems phase segregate. We have carried out a quantitative analysis of the local dielectric constant for charged-neutral diblock copolymer melts using field-theoretic simulations based on the self-consistent field theory (SCFT). Quantitative expression for the local dielectric constant in terms of the local electric field will be presented along with its effects on the microphase separation in these systems. Using large-scale SCFT simulations, we will explore the effects of different experimental parameters on the morphology diagram. These parameters include the chain length, temperature, degree of ionization and length fraction of the charged block. Also, the effect of added salt on the disorder-order transition temperature and the domain spacings of the ordered morphologies along with the distribution of small ions (counterions and co-ions) will be presented.

Rajeev Kumar
National Center for Computational Sciences,
Oak Ridge National Lab, Oak Ridge, TN- 37831

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