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Stabilization of Bicontinuous Phases in Diblock Copolymer Systems FERNANDO ESCOBEDO, FRANCISCO MARTINEZ-VERACOECHEA, Cornell University — We used a coarse-grained description of the copolymer chains (i.e., dissipative particle dynamics fluid), together with continuum-space Monte Carlo and Molecular Dynamics methods, to study systems of diblock copolymers melts that have been "filled" with selective additives (i.e., homopolymer, and nanoparticles). Approximate phase boundaries were found via free-energy calculations. We focus on the stabilization of bi-continuous phases and the strikingly different phase behavior observed when the nature of the selective filler is changed. Our results elucidate the origins of the packing frustration that limits the viability of the gyroid, double-diamond, and plumber's nightmare phases and provide insights for overcoming it. Attention is also focused on directly determining the areas of phase diagram where macro- phase separation occurs. We compare the particle-based simulation results with the results obtained by means of self- consistent filed theory calculations.

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