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Simulation of free energies of bicontinuous morphologies formed through block copolymer/homopolymer self-assembly POORNIMA PADMANABHAN, Cornell University, FRANCISCO MARTINEZ-VERACOECHEA, None, FERNANDO ESCOBEDO, Cornell University — Different types of bicontinuous phases can be formed from A-B diblock copolymers by the addition of A-type homopolymers over a range of compositions and relative chain lengths. Particle-based molecular simulations were used to study three bicontinuous phases – double gyroid (G), double diamond (D) and plumber's nightmare (P) - near their triple point of coexistence. For 3-D ordered phases, the stability of the morphology formed in simulation is highly sensitive to box size whose exact size is unknown a-priori. Accurate free energy estimates are required to ascertain the stable phase, particularly when multiple competing phases spontaneously form at the conditions of interest. A variant of thermodynamic integration was implemented to obtain free energies and hence identify the stable phases and their optimal box sizes by tracing a reversible path that connects the ordered and disordered phases. Clear evidence was found of D-G and D-P phase coexistence, consistent with previous predictions for the same blend using Self-consistent field theory. Our simulations also allowed us to examine the microscopic details of these coexisting bicontinuous phases and detect key differences between the microstructure of their nodes and struts.

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None

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