Abstract Submitted
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Using thermodynamic integration to simulate the free-energy of bicontinuous phases formed by block copolymer/homopolymer blends POORNIMA PADMANABHAN, Cornell University, FRANCISCO MARTINEZ-VERACOECHEA, Infochem Computer Services Ltd., UK, FERNANDO ESCOBEDO, Cornell University — AB diblock copolymers can co-assemble with A-type homopolymers to form different bicontinuous phases whose 3D connectivity of both A and B domains is of interest for potential applications in nanolithography, photovoltaic cells and drug delivery. In this work, we use particle-based simulations to study the vicinity of a triple point where three bicontinuous phases (gyroid, double diamond and plumber's nightmare) were predicted to coexist by Self Consistent Field Theory. A key roadblock is that bicontinuous morphologies are highly sensitive to the commensurability of the simulation box size and the a-priori unknown unit cell size. Accurate estimation of free energies is thus crucial to the determination of the stable morphology. In this work, we apply thermodynamic integration over a constructed reversible path to calculate the free energies of these bicontinuous phases relative to a disordered phase and compare the predicted phase stability to results from alternative methods.

Poornima Padmanabhan
Cornell University

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