The Impact of Polydispsersity on the Tethereed Nanosphere Phase Diagram

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Recent simulations predict that aggregating nanospheres functionalized with polymer "tethers" can self-assemble to form a cylinder, perforated lamallae, lamallae, and even the double gyroid phase also seen in block copolymer and surfactant systems. We study the impact of nanoparticle size polydispersity on the properties of the phase diagram. We show that in the portions of the phase diagram characterized by an icosahedral packing motif, a low amount of polydispersity lowers the energy and a large amount of polydispersity raises the potential energy of the system by disrupting the icosahedral packing. In the portions of the phase diagram characterized by crystalline packing, polydispersity raises the energy of the system and induces a phase transition from crystalline to liquid within the nanosphere packing of the microphase.