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Mesophases of soft-sphere aggregates HOMIN SHIN, GREGORY GRASON, CHRISTIAN SANTANGELO, University of Massachusetts, Amherst — Soft spheres interacting via a hard core and purely repulsive shoulder self-assemble into clusters forming a variety of mesophases. We combine a mean field theory developed from a lattice model with a level surface analysis of the periodic structures of soft-sphere aggregates to study stable morphologies for a class of interaction potentials. The mean-field solution shows that the site occupation density and interparticle potential are self-consistently related to an “effective field” acting on each particle. In the strong segregation limit, the space group symmetry of possible aggregate structures associated with the spatially modulated field, together with a half-filling condition at the interface of morphology, allows us to produce a phase diagram including Lamella, Hexagonal-columnar, and BCC phases, and their inverse phases in the parameter space of chemical potential and interparticle potential. Finally, we discuss the finite-temperature corrections to strong segregation theory in terms of Sommerfeld-like expansion and how these corrections affect the thermodynamic stability of bicontinuous mesophase structures, such as gyroid.

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