Abstract Submitted
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Mesophase behavior and effect of polydispersity in assemblies of polyhedral particles[1] FERNANDO ESCOBEDO, UMANG AGARWAL, Cornell University — Mesophase behavior of polyhedral particles is uniquely linked to the inherent interactions embedded in their geometrical shape. A two-parameter model based on particle shape anisotropy and order of symmetry has been proposed for predicting phase behavior of polyhedral particles. The focus of the current work is to explore the phase behavior of a distinct class of polyhedral shapes, which emerge at different growth stages of PbSe nanocrystal formation. The body of knowledge that is emerging from these studies may prove useful in designing optimal self-assembly strategies for many desired nanostructures; e.g., as in our ongoing efforts in understanding the nanocrystal superlattice formation for solar cell applications. Moreover the effect of particle size polydispersity is explored by simulating the assembly of two representative shapes exhibiting totally different mesophase behavior. It is found that while mesophases are quite resilient to particle size anisotropy, the ordered structures are a complex function of the polydispersity and geometric attributes.

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