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Predictive Self-Assembly of Complex Crystals via Building Block Design

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A primary challenge for the development of bulk, scalable, and high yield materials with interesting properties is the limited number of structures that can be obtained via self-assembly of nano and micrometer sized particles. Systematic and extensive computational studies of hard polyhedral particles have demonstrated that anisotropy of the building blocks can be a viable route for increasing variability of assembled patterns [1, 2, 3]. Interestingly, the types of structures assembled from this method were shown to be predictable from information contained already in the dense fluid, prior to crystallization. In this talk, the role of such local structures for self-assembly will be rationalized and we will demonstrate how this information can be used as a strategy for design of crystalline and quasicrystalline patterns for both symmetric and asymmetric particles.

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