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Binary mixtures of polyhedral nanoparticles: from phase separation to superstructures MIHIR KHADILKAR, UMANG AGARWAL, FERNANDO ESCOBEDO, Cornell University — Polyhedral nanoparticles have emerged as important model systems for both fundamental studies of entropic self-assembly as well as material design. The mixing of more than one shape provides a promising strategy towards achieving a greater variety of structures and properties. We explore this with the study of the phase behavior of binary mixtures of hard convex polyhedra having similar sizes but different shapes. Choosing representative particle shapes from those readily synthesizable, we find that the phase behavior of such mixtures is dependent on the interplay of mixing and packing entropy, which can give rise to miscible or phase-separated states. While expectedly many of the binary systems studied exhibit phase separation at high pressures due to the incompatible pure-component crystal structures, our study shows that the essential qualitative trends in miscibility and phase separation can be correlated to properties of the pure components, such as the relative values of the order-disorder transition pressure of each component. However, the relative size ratios and the presence of mesophases for the pure-component systems are also critical in aiding the formation of fully miscible blends of novel plastic crystalline superstructures.

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