Electronic Supplementary Information for: Tunable Assembly of Host–Guest Colloidal Crystals

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Beginning of Supplementary Figures



Figure S1: Structural analysis of self-assembled host-guest systems. Each row corresponds to a system with a specific guest shape shown in the inset in the middle column. Left columns: distributions of body orientations of host and guest particles for systems shown in Figs. 2 and 4 in the main text. Middle columns: distributions of the hexatic bond orientational order parameter ψ_j for host and guest particles. For the host we assumed 3 nearest neighbors and for the guests 6 nearest neighbors. Right columns: spatial correlation functions of body orientations of host and guest particles. Data for each distribution (correlation function) was collected from (averaged over) the final 5×10^6 steps of the simulation.



Figure S2: Snapshot of a system containing only hard star particles at $P^* = 3.5$ showing that hexamer pores do not assemble in the absence of guest particles.



Figure S3: Tiling the plane with hexameric shield-shaped pores results in hexagon pores. To illustrate this we place a single shield pore and then add additional shield pores (number denoting the number of shield pores) with edge–edge connections that make more shield pores. Placing three shield pores in this way results in an additional emergent shield pore shown in 3. However, placing a 4th shield pore results in the emergence of a hexagon pore, indicating that hexamer shield pores alone cannot tile space.