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Self-limited self-assembly of chiral filaments[1] MICHAEL HAGAN, YASHENG YANG, ROBERT MEYER, Brandeis University — The assembly of filamentous bundles with controlled diameters is common in biological systems and desirable for the development of nanomaterials. We discuss dynamical simulations and free energy calculations on patchy spheres with chiral pair interactions that spontaneously assemble into filamentous bundles. The chirality frustrates long-range crystal order by introducing twist between interacting subunits. For some ranges of system parameters this constraint leads to bundles with a finite diameter as the equilibrium state, and in other cases frustration is relieved by the formation of defects. While some self-limited structures can be modeled as twisted filaments arranged with local hexagonal symmetry, other structures are surprising in their complexity. We discuss the relation between model structures and finite bundles in biological or biomaterials systems, and implications for the design of nanostructured materials with controlled sizes.

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