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Why (almost) all bundles are chiral[1] ZACHARY V. KOST-SMITH, ROBERT A. BLACKWELL, MATTHEW A. GLASER, Univ of Colorado - Boulder — We examine the self assembly of bundles of achiral hard rods with distributed, short-range attractive interactions. We show that in the majority of cases the equilibrium state of the bundle is chiral, with a double twist structure. We use biased Monte Carlo techniques and cell theory to compute the free energy as a function of an appropriately defined twist order parameter, and show that the formation of spontaneously chiral bundles is driven by maximization of orientational entropy. The finite curvature of the bundle boundary permits *orientational escape*, in which the circumferential angular range of motion of the rods is maximized for some finite average tilt. We map out the phase diagram of bundles in terms of the density, the ratio of rod length to bundle radius, L/R, and rod aspect ratio, L/D, and find transitions between untwisted, weakly twisted, and strongly twisted states. This work helps explain the common observation of twisted macroscopic bundles, and may provide insight into observations of twist in self-assembled membranes of colloidal rods.[2]

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[2]Reconfigurable self-assembly through chiral control of interfacial tension, Nature, 481:348-351, Jan 2012

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