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Simulation of the liquid crystalline behavior of cuboidal colloidal particles BETTINA JOHN, ABRAHAM STROOCK, FERNANDO ESCOBEDO, Cornell University — The effect of the shape of colloidal particles on their liquid-crystalline bulk-phase behavior was investigated in this work. The particles considered have a cuboidal shape with axes lengths a = b $\neq$ c and experience purely repulsive (hard-core) interactions. These particles exhibit marked self-assembly properties because of their flat facets and square edges. Monte Carlo simulations at constant osmotic pressure were used to map out the lyotropic phase diagram of such hard particles. For cubical particles (i.e., with c=a), a liquid-crystalline phase known as cubatic phase forms at intermediate concentrations. Such a mesophase exhibits orientational ordering along three axes (cubatic order) but significant translational disorder. The isotropic-to-cubatic phase transition was found to be first order and be driven by the interplay of orientational and packing entropy. The onset and stability of the cubatic phase was little affected by the roughness of the cuboid surfaces and by moderate size polydispersity. The phase diagrams were also mapped out for cuboidal particles with aspects ratios ranging from c:a=1:3 to c:a=8:1. As expected, the phase behavior of long cuboidal rods approaches that of spherocylinders of similar aspect ratios; e.g., nematic and smectic phases were observed for c:a=8:1 while only the smectic phase is observed for c:a=5:1. The cubatic phase was prominent at c:a in the range of 1 to 4.

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