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Mesophase Assembly of Nanoscale Prisms ZIWEI WANG, Northwestern University, ZIHAO OU, QIAN CHEN, University of Illinois Urbana-Champaign, ERIK LUIJTEN, Northwestern University — Predicting structures self-assembled from basic building blocks remains a central problem in materials design and engineering. Entropy-driven packing behavior has been studied extensively via simulations of hard objects. However, in many experimental systems intrinsic, highly anisotropic interactions play an important role as well, and can overwhelm the entropic effects of shape, especially on the nanoscale. As a result, omission of enthalpic effects in large-scale simulations leaves many essential mesophases unexplored. We perform Monte Carlo simulations of nanoscale prisms with properly modeled interactions, and demonstrate that these give rise to a novel plastic-crystal mesophase of prisms stacked with random in-plane orientations, organized on a 2D hexagonal lattice. These simulations explain direct experimental observations performed with liquid-phase transmission electron microscopy.

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