493h Self-Assembly of Polymer-Tethered Nanorods

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The need to organize nanoparticles into complex structures for applications ranging from electronics to solar energy utilization has focused increasing attention on the method of self assembly, whereby material building blocks self-organize into patterns based on thermodynamic principles. We performed molecular simulations to predict the phases formed by self-assembly of rod-like nanoparticles functionalized by a single polymer "tether" attached to the rod end. Microphase separation of the immiscible tethers and nanorods coupled with the liquid crystal ordering of the rods induces the formation of a smectic C phase, a 3-D tetragonally perforated lamellar phase and a honeycomb phase; the latter two have been observed experimentally but have not been predicted by any theory or previous simulations[1]. We also predict a new phase – a racemic mixture of hexagonally-arranged chiral cylinders that self-assemble from achiral building blocks.

[1] Horsch, M.A. et al. Self-Assembly of Polymer-Tethered Nanorods. (under review)