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Design Rules for Ordered SAMs on Patchy Nanoparticles AARON SANTOS, SHARON GLOTZER, University of Michigan — Recently, the self-assembly of ordered stripe-like domains of ligands on the surface of spherical nanoparticles was reported. Molecular ligands tethered to nanoparticle surfaces play an important role in the self-assembly of many systems. These tethers contribute significantly to the free energy of the system because of their large conformational entropy. In general, the stable state can be determined by minimizing the free energy of the system. We have developed a coarse-grained model to rapidly simulate the phase separation of ligands on a surface. The model uses mean field and two-body approximations to compute the conformational entropy of tethers. Using these approximations, one can quickly compute the phase diagrams using a simple Metropolis Monte Carlo simulation. In contrast to traditional coarse-grained simulation methods, which can take hundreds to thousands of hours of CPU time, our coarse-grained model can generally find free energy minimum states in under a few hours. We use this model to study the self-assembly of monolayers on nanoparticle surfaces into a variety of patterns and predict design rules for assembling patchy particles. This work has profound implications for the design and synthesis of ordered patchy particles.

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