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Role of Polymer-grafted Nanoparticle Interactions in Supercrystal Self-Assembly[1] NATHAN HORST, CURT WALTMANN, Department of Materials Science and Engineering, Iowa State University and Ames Lab, ALEX TRAVESSET, Department of Physics and Astronomy, Iowa State University and Ames Lab
— Many successful strategies are available for the programmable self-assembly of nanoparticle superlattices. In this talk, we discuss the the case of nanoparticles with grafted polymer ligands. For very short polymers, the phase diagram is rationalized by borrowing results from hard-sphere packing models. Although a clear correlation exists between the maximum of the packing fraction of hard spheres and supercrystal equilibrium phases found experimentally, these systems are flexible, which leads to clear deviations from the sphere packing model. Using theoretical and computational models, we present an investigation of the interactions of polymer-grafted nanoparticles, focusing on the role of the rigidity of the chain, and how it affects the resulting two and three-dimensional superlattice structures. Comparison with an experimental system of gold nanoparticles grafted with polyethylene glycol is also presented.

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