

Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Polymer Conformation and Topological Defects in Systems of Hairy and DNA hybridized Nanoparticles CHRIS KNOROWSKI, ALEX TRAVESSET, Iowa University Department of Physics and Astronomy and Ames Lab — Systems of hairy and DNA hybridized Nanoparticles are able to self-assemble into an array of superlattices. Understanding the role the polymer plays is critical to predicting the superlattice structure. In this talk, we use Molecular Dynamics to study hairy nanoparticles where the grafted polymer is modeled explicitly. We study self-assembly starting from a liquid and following the nucleation and growth of large nanoparticle superlattices (2000NP). We explore the role of polymer stretching as well as the geometric frustration of the polymer for both spherical and cubic nanoparticles. We also provide a characterization of the dynamics, including topological defects. Further, we will discuss the difficulties and methods for simulating large lattices in molecular dynamics.

Chris Knorowski
Iowa University Department of Physics and Astronomy and Ames Lab

Date submitted: 15 Nov 2013

Electronic form version 1.4