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Topological Defects and Structure Prediction in Nanoparticle Superlattices[1] ALEX TRAVESSET, NATHAN HORST, CURTIS WALTMANN, SURYA MALLAPRAGADA, HONGHU ZHANG, Iowa State University and Ames lab, WENJIE WANG, Ames lab, DAVID VAKNIN, Iowa State University and Ames lab — Materials whose fundamental units are nanoparticles, instead of atoms or molecules, are gradually emerging as major candidates to solve many of the technological challenges of our century. Those materials also display unique structural, dynamical and thermodynamical properties, often reflecting deep underlying geometry and topological constraints. In this talk, I will focus on crystalline assemblies of nanoparticles, i.e. supercrystals. I will discuss the challenges to predict the structure and dynamics of supercrystals and discuss our computational and analytical approach to predict two successful experimental strategies for the rational design of nanoparticle materials: evaporation of organic solvents with nanoparticles having hydrocarbon as capping ligands, and a new strategy developed at Ames lab consisting of crystallization of nanoparticle neutral (uncharged) polymer brushes by induced electrostatic phase separation.

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