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Prediction of Binary Nanoparticle Superlattices from Soft Potentials[1] NATHAN HORST, Department of Materials Science and Engineering, Iowa State University, ALEX TRAVESSET, Department of Physics and Astronomy, Iowa State University — Driven by the hypothesis that a sufficiently continuous short-ranged potential is able to account for shell flexibility and phonon modes and therefore provides a more realistic description of nanoparticle interactions than a hard sphere model, we compute the solid phase diagram of particles of different radii interacting with an inverse power law potential. We explore 24 candidate lattices where the p-exponent, determining the short-range properties of the potential, is varied between p=12 and p=6, and optimize the free energy with respect to additional internal parameters. The phase diagrams contain the phases found in ongoing self-assembly experiments, including DNA programmable self-assembly and nanoparticles with capping ligands assembled by evaporation from an organic solvent. The resulting phase diagrams can be mapped quantitatively to existing experiments as a function of only two parameters: nanoparticle radius ratio (γ) and softness asymmetry (SA).

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Nathan Horst
Department of Materials Science and Engineering, Iowa State University

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