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DNA-linked NanoParticle Lattices with Diamond Symmetry: Stability and Shape HAMED EMAMY, Wesleyan University, Physics Department, ALEXEI TKACHENKO, OLEG GANG, Brookhaven National Laboratory, Center for Functional Nanomaterials, FRANCIS STARR, Wesleyan University, Physics Department — The linking of nanoparticles (NP) by DNA has been proven to be an effective means to create NP lattices with specific order. Lattices with diamond symmetry are predicted to offer novel photonic properties, but self-assembly of such lattices has proven to be challenging due to the low packing fraction, sensitivity to bond orientation, and local heterogeneity. Recently, we reported an approach to create diamond NP lattices based on the association between anisotropic particles with well-defined tetravalent DNA binding topology and isotropically functionalized NP. Here, we use molecular dynamics simulations to evaluate the Gibbs free energy of these lattices, and thereby determine the stability of these lattices as a function of NP size. The lattice free energy has a minimum for NP size near 50 nm, and rapid increases for larger NP, destabilizing the lattice. We also predict the equilibrium shape for the cubic diamond crystallite using the Wulff construction method. Specifically, we predict the equilibrium shape using the surface energy for different crystallographic planes. We evaluate surface energy directly form molecular dynamics simulation, which we correlate with theoretical estimates from the expected number of broken DNA bonds along a facet.

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