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DNA-linked NanoParticle Lattices with Diamond Symmetry: Stability, Shape and Optical Properties HAMED EMAMY, Wesleyan Univ, ALEXEI TKACHENKO, Brookhaven National Laboratory, OLEG GANG, Columbia Univ, FRANCIS STARR, Wesleyan Univ — 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 and DNA stiffness. 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. Furthermore we study the optical properties of this structure, e.g optical bandgap.

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