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Relative Stability of DNA-Linked Nanoparticle Crystals FERNANDO VARGAS LARA, FRANCIS STARR, Wesleyan University — The creation of three-dimensional, crystalline ordered nanoparticle (NP) structures linked by DNA has proved experimentally challenging. Here we aim to systematically study parameters that influence the relative thermodynamic stability of such crystals. We carry out molecular dynamics simulations of a coarse-grained model in which DNA strands are tethered to a core icosahedral NP and examine the influence of strand length, fraction of linking bases in the strand, and strand stiffness on crystal stability. We use the thermodynamic integration method to compute the free energy, entropy, and melting point for BCC and FCC lattices formed for a broad range of parameter choices. We rationalize our findings using a simple model for the entropy difference due to hybridization, which suggests that the stability, measured by the heat of melting, can be expressed as a simple function of the fraction of linking base pairs.

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