Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Stability of DNA-linked Nanoparticle Crystals: Effect of Number of Strands OLIVIA PADOVAN-MERHAR, FERNANDO VARGAS LARA, FRANCIS STARR, Physics Dept, Wesleyan University, Middletown CT — Three-dimensional lattices of DNA-functionalized nanoparticles (NP) have potential application to novel devices and materials, but most experimental attempts to form crystals result in amorphous packing. Molecular models of DNA-functionalized NP have focused mainly on a small ($\sim$10) number of DNA strands, while the experimental particles have a large ($>$50) number of attached strands. Here we study crystal formation of DNA-linked NP using a coarse-grained molecular model in which ssDNA are attached to spherical core NP. We examine the effect of strand number on crystal stability by using the method of thermodynamic integration to compute the free energy and entropy of BCC and FCC lattices, as well as determine the thermodynamic melting point of these structures. Additionally, it has been argued that the surface of gold NP have significant mobility, possibly resulting in DNA tethers which are not localized at specific points on the NP surface. We show that such strand mobility results in a crystal that is less stable than one formed when strands are rigidly attached.

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Date submitted: 20 Nov 2009 Electronic form version 1.4