Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Modeling of DNA-Directed Colloidal Self-Assembly and Crystallization TING LI, RASTKO SKNEPNEK, ROBERT J. MACFARLANE, CHAD A. MIRKIN, MONICA OLVERA DE LA CRUZ, Northwestern University — A series of design rules have recently been developed for using gold nanoparticles conjugated with a dense layer of double stranded DNA chains to assemble a wide variety of nanoparticle superlattice structures [1]. Key design parameters for obtaining different structures in a binary system were shown to be the ratio of the hydrodynamic radii of the DNA-conjugated particles, the ratio of the number of DNA strands per particle, and the self- or non-self-complementary nature of the DNA sequences guiding the assembly process. Guided by those experiments, we have built a coarse grained model that faithfully mimics relative design parameters in the experimental system. Working with nanoparticles in the size range from 8nm to 15nm, overall DNA-nanoparticle hydrodynamic radii of 10nm to 30nm, and the number of DNA strands per particle between 30 and 100, we have developed a simulation method that confirms that these design rules can be used to assemble a variety of different crystal structures. In particular, we have identified FCC, BCC, CsCl, AlB_2 and Cr_3Si structures. With these data, we have constructed a detailed phase diagram that closely corresponds to the experimentally obtained phase diagram developed in ref. [1]. [1] R. J. Macfarlane, B. Lee, M. R. Jones, N. Harris, G.

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Date submitted: 11 Nov 2011 Electronic form version 1.4