

Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Modelling of DNA-Mediated of Two- and –Three dimensional Protein-Protein and Protein-Nanoparticle Self-Assembly JAIME MILLAN, JANET MCMILLAN, JEFF BRODIN, Northwestern University, BYEONGDU LEE, Argonne National Laboratory, CHAD MIRKIN, MONICA OLVERA DE LA CRUZ, Northwestern University — Programmable DNA interactions represent a robust scheme to self-assemble a rich variety of tunable superlattices, where intrinsic and in some cases non-desirable nano-scale building blocks interactions are substituted for DNA hybridization events. Recent advances in synthesis has allowed the extension of this successful scheme to proteins, where DNA distribution can be tuned independently of protein shape by selectively addressing surface residues, giving rise to assembly properties in three dimensional protein-nanoparticle superlattices dependent on DNA distribution. In parallel to this advances, we introduced a scalable coarse-grained model that faithfully reproduces the previously observed co-assemblies from nanoparticles and proteins conjugates. Herein, we implement this numerical model to explain the stability of complex protein-nanoparticle binary superlattices and to elucidate experimentally inaccessible features such as protein orientation. Also, we will discuss systematic studies that highlight the role of DNA distribution and sequence on two-dimensional protein-protein and protein-nanoparticle superlattices.

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Date submitted: 11 Nov 2016

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