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Modeling of DNA-Mediated Self-Assembly from Anisotropic Nanoparticles: A Molecular Dynamics Study JAIME MILLAN, MARTIN GIRARD, JEFFREY BRODIN, MATT O'BRIEN, CHAD MIRKIN, MONICA OLVERA DE LA CRUZ, Northwestern University — The programmable selectivity of DNA recognition constitutes an elegant scheme to self-assemble a rich variety of superlattices from versatile nanoscale building blocks, where the natural interactions between building blocks are traded by complementary DNA hybridization interactions. Recently, we introduced and validated a scale-accurate coarse-grained model for a molecular dynamics approach that captures the dynamic nature of DNA hybridization events and reproduces the experimentally-observed crystallization behavior of various mixtures of spherical DNA-modified nanoparticles. Here, we have extended this model to robustly reproduce the assembly of nanoparticles with the anisotropic shapes observed experimentally. In particular, we are interested in two different particle types: (i) regular shapes, namely the cubic and octahedral polyhedra shapes commonly observed in gold nanoparticles, and (ii) irregular shapes akin to those exhibited by enzymes. Anisotropy in shape can provide an analog to the atomic orbitals exhibited by conventional atomic crystals. We present results for the assembly of enzymes or anisotropic nanoparticles and the co-assembly of enzymes and nanoparticles.

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