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Hybridization dynamics to DNA guided crystallization[1] TING LI, Northwestern University, RASTKO SKNEPNEK, Syracuse University, MONICA OLVERA DE LA CRUZ, Northwestern University, NORTHWESTERN UNIVERSITY TEAM — DNA recognition inspires an elegant protocol to design versatile nanoparticle assemblies. Although great achievements in DNA programmed periodic structures have been obtained, it took over a decade to realize even the basic crystal structures like FCC and BCC in an experiment. We use molecular dynamics simulations to discuss the dynamic aspects of the assembly process and identify ingredients that are key to successfully assemble nanoparticle superlattices through DNA hybridizations. The scale-accurate coarse-grained model [1,2] faithfully captures the relevant dynamics of the DNA hybridization, and is able to recover the in situ formation of all to date experimentally reported binary superlattices (BCC, CsCl, AlB2, Cr3Si and Cs6C60 lattices). We used a multi-scale simulation approach to study the assembly mechanism in systems with up to 10^6 degrees of freedom and found that the assembly process is enthalpy-driven. Finally, we investigated the optimal strength of DNA linkers, hybridization dynamics, and percentage of hybridizations for different binary systems. Based on these results, we suggest a protocol for future nanomaterial designs with versatile DNA interactions. [1] Knorowski, C., et al. P.R.L. 2011,106,215501; [2] Li, T.I.N.G., et al. Nano Letters 2012,12,2509.

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