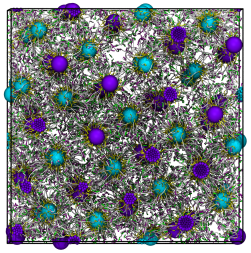

Thermally Active Hybridization Drives the Crystallization of DNA-functionalized Nanoparticles

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We used molecular dynamics simulations to analyze dynamic aspects of the assembly process and identify ingredients that are key to a successful assembly of nanoparticle superlattices through DNA hybridization. A scale-accurate coarse-grained model with explicit DNA chains faithfully captures the relevant contributions to the kinetics of the DNA hybridization process, and is able to recover all experimentally reported to date binary superlattices (BCC, CsCl, AlB_2, Cr_3Si, and Cs_6C_{60}). We found that the optimal range of the DNA linker interaction strengths for a successful assembly is $12-16k_BT$ and the optimal mean lifetime of a DNA hybridization event is $10^{-4}-10^{-3}$ of the total time it takes to form a crystal. We also obtained the optimal percentage of hybridized DNA pairs for different binary systems. Based on these results, we proposed suitable linker sequences for future nanomaterials design.

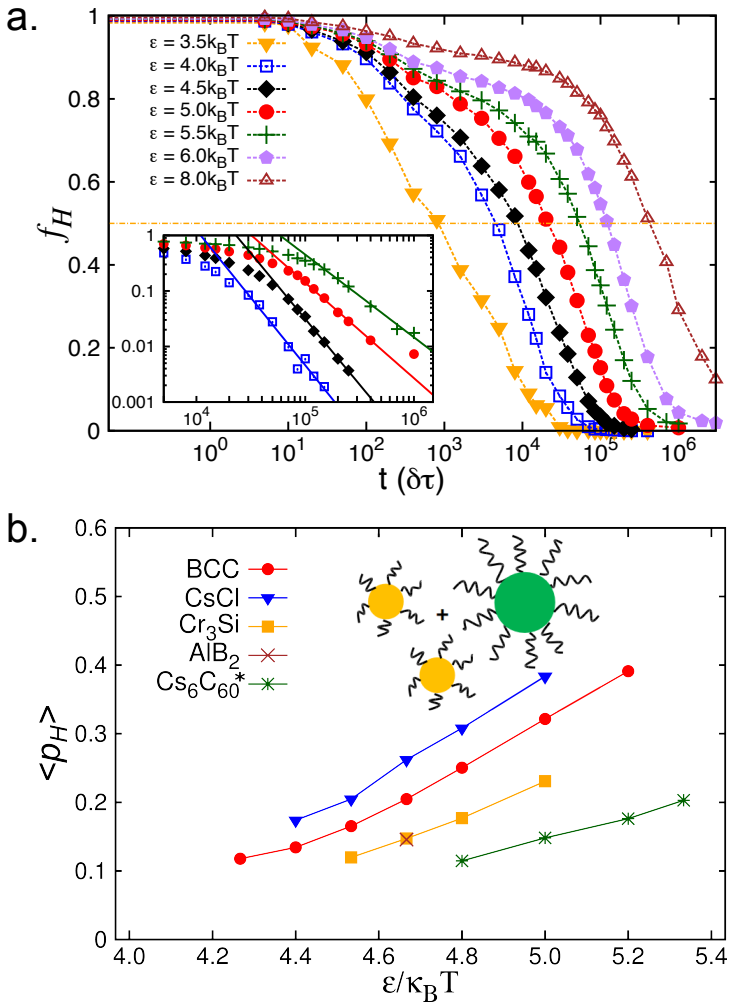

Figure: (a) Fraction of hybridizations f_H that survive up to a time t. (b) Optimal linker strength 3×ε and corresponding percentage of hybridized DNA pairs $<p_H>$ for various binary systems.

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