Modeling the Crystallization of Spherical Nucleic Acid Nanoparticle Conjugates with Molecular Dynamics Simulations

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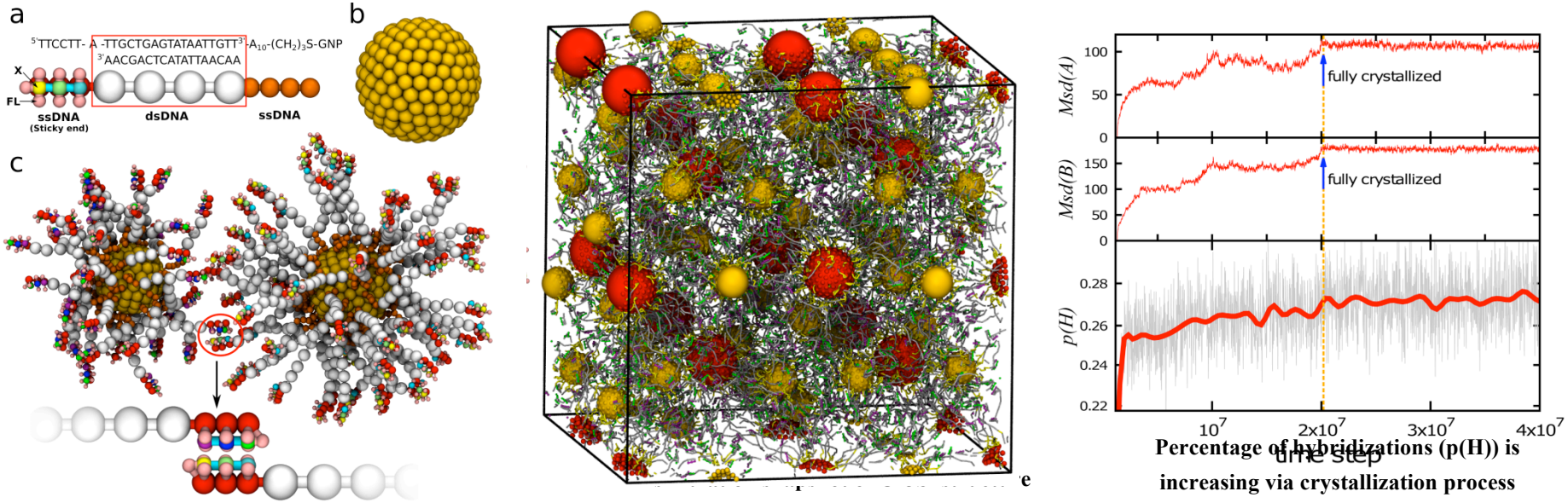
A series of design rules have recently been developed for using spherical nucleic-acid (SNA) gold nanoparticle conjugates to assemble a wide variety of nanoparticle superlattice structures [1]. To better design and predict novel assemblies prior to an experimental realization, we have extended the coarse grained model of Knorowski et al. [2] to faithfully mimic relative design parameters in this dsDNA system. We worked on Molecular Dynamics simulations 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 40 and 100, the model proves robust such that completely random initial configurations can self-assemble into a variety of crystal structures, including BCC, CsCl, AlB_2 and Cr_3Si.



Percentage of hybridizations (p(H)) is increasing via crystallization process

With these simulation data, we have constructed detailed phase diagrams that closely correspond to the experimental results from wet-laboratory studies [1]. In addition, by tracking the in-situ movements of nanoparticles and monitoring the attachment and detachment events of complementary DNA linkers via the self-assembly process, we provide discussion on the key ingredients for a successful crystallization: We showed that highly dynamic hybridization processes between the semiflexible grafted chains enables crystallization.

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[1] Macfarlane, R. J.; Lee, B.; Jones, M. R.; Harris, N.; Schatz, G. C.; Mirkin, C. A. *Science* **2011**, 334, 204–208. [2] Knorowski, C.; Burleigh, S.; Travesset, A. *PRL* **2011**, 106, 215501.