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Self-assembly and Evolution from protein complexes to DNA nanostructures

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The remarkable ability of biological matter to robustly self-assemble into well defined composite objects excites the imagination, suggesting that these processes could perhaps be emulated through the judicious design of synthetic building blocks. We use statistical mechanics to uncover the design rules for self-assembly into well defined three dimensional composite objects. In Nature, the rules for self-assembly emerge from an evolutionary process. We show how some patterns in protein complexes can be explained by their evolutionary origin [1]. We also introduce a coarse-grained rigid nucleotide model of DNA that reproduces the basic thermodynamics of short strands: duplex hybridization, single-stranded stacking and hairpin formation, and also captures the essential structural properties of DNA: the helical pitch, persistence length and torsional stiffness of double-stranded molecules, as well as the comparative flexibility of unstacked single strands [2]. We apply the model to calculate the detailed free-energy landscape of one full cycle of DNA "tweezers," a simple machine driven by hybridization and strand displacement. We also study other nanomachines as well as processes such as force-induced melting, cruciform formation and the self-assembly of DNA tetrahedra.

[1] The self-assembly and evolution of homomeric protein complexes Gabriel Villar, et al., Phys. Rev. Lett. 102, 118106 (2009
[2] Structural and thermodynamic properties of a coarse-grained model of DNA, Thomas E. Ouldridge, Ard A. Louis, Jonathan P.K. Doye, J. Chem. Phys. 134 , 085101 (2011)