Title: Self-assembly of DNA Coated Colloids: Theory and Computer Simulations

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Abstract

Self-assembly is a spontaneous organization of components often in the form of higher-order structures. Self-assembled structures are abundant in nature, and their functionality tends to be structure specific. Designing functional materials of specific symmetry, controlled hierarchy, and directionality via self-assembly process using either natural/synthetic/hybrid materials as building blocks is an emerging field of chemistry, physics, and materials sciences [1]. Such self-assembled systems have a wide range of technological applications in thin-film transistors, bio-sensing, photonic crystals etc. My research interests revolve around structure formation using DNA-coated colloids [2-3], self-assembly of lipophilic molecules [4-5], and rheological studies of soft matter [6].

In this talk, I will highlight the demands of advanced simulation approaches developed based on statistical mechanics for exploring self-assembly systems made of DNA coated spherical colloids. I will show how the DNA coated colloids (Figure 1a) can be used to control the growth of crystals (Figure 1b and c) and the microscopic mechanism of their relaxation processes (Figure 1d) [2,3]. Brownian dynamics coupled with Gillespie Algorithm on a sophisticated coarse-grained model and a mean-field theory are employed in this work. I will also discuss the kinetic bottlenecks in the assembly process of DNA mediated interactions. The developed techniques could be useful not only for DNA-coated colloids but also to investigate the dynamics of systems feature ligand-receptor interactions.

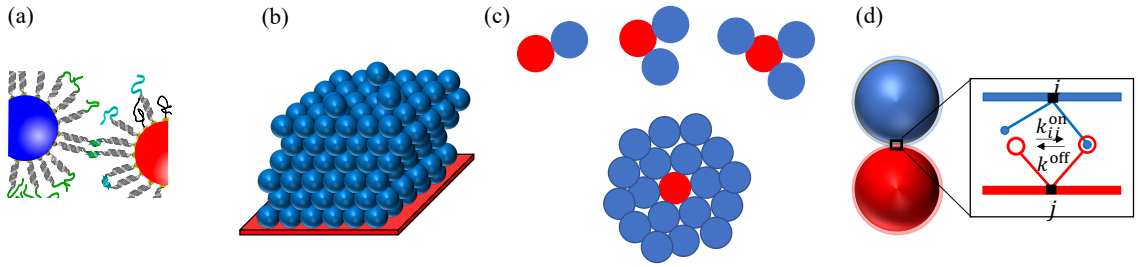

Figure 1. (a) DNA coated colloids. Structure formation in a controlled manner using DNA mediated interactions (b) from a functionalized surface and (c) in solution. (d) Microscopic dynamics of DNA coated colloids.

References

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