Programmable self-assembly of DNA-nanoparticle mesostructures

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In recent years, an impressive progress has been made in using the molecular recognition properties of DNA to control self-assembly of nanoparticles (NPs) into variety of DNA-NP supercrystals. Self-assembly of finite size DNA-NP structures have received much less attention. Such programmable NP clusters would open new opportunities in a variety of fields where bottom-up assembly of 3D nano-objects with well defined composition and architecture is required, e.g. nanoplasmonics, nanomedicine, metamaterials. In my talk, I will show that a variety of target mesoscopic structures, each with a programmed local morphology and complex overall shape, can be self-assembled at a near perfect yield. The proposed building blocks, octopus NPs, are inspired by recent proof-of-principle experiments in which DNA were attached at specific locations on the particles. We introduce the methodology for solving the inverse problem in self-assembly, i.e. designing building blocks that assemble into an arbitrary desired structure, in a robust manner. The design method is then verified by simulating the self-assembly of cubes, pyramids and even an Empire State Building model from an initially homogeneous solution of NPs. Our study demonstrates that one can completely avoid unwanted metastable configurations, and therefore the self-assembly occurs on relatively fast timescales determined primarily by particle diffusion and binding, but not by exploration of potentially vast configurationally space (as e.g. in protein folding problem).