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Inverse Problem in Self-assembly[1]

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By decorating colloids and nanoparticles with DNA, one can introduce highly selective key-lock interactions between them. This leads to a new class of systems and problems in soft condensed matter physics. In particular, this opens a possibility to solve inverse problem in self-assembly: how to build an arbitrary desired structure with the bottom-up approach? I will present a theoretical and computational analysis of the hierarchical strategy in attacking this problem. It involves self-assembly of particular building blocks ("octopus particles"), that in turn would assemble into the target structure. On a conceptual level, our approach combines elements of three different brands of programmable self assembly: DNA nanotechnology, nanoparticle-DNA assemblies and patchy colloids. I will discuss the general design principles, theoretical and practical limitations of this approach, and illustrate them with our simulation results. Our crucial result is that not only it is possible to design a system that has a given nanostructure as a ground state, but one can also program and optimize the kinetic pathway for its self-assembly.

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