Programmable Nanoscale Materials

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The diverse emerging nanotechnological applications, from photonics to biomaterials and from computing to energy, require creating complex 3D-engineered architectures to enable novel functions. The limitations of traditional top-down fabrication methods prevent the realization of concepts that require complex 3D nanostructures. While self-assembly approaches demonstrate the diversity of spontaneously forming structures, they typically cannot provide structural designability and universality for system formation since assembly is sensitive to components' characteristics. This coupling between the nature of nanocomponents and their assembly behavior makes it difficult to employ self-assembly as a nanofabrication methodology.

To overcome these challenges, we developed an inverse design strategy based on the programmability of DNA interactions and control of their nanoscale architectures for creating 3D lattices with an arbitrary prescribed organization of nanocomponents. We demonstrated that diverse inorganic and biomolecular nanocomponents can be hosted by such lattices with designed organization, thus decoupling the assembly process from the nature of these nanocomponents. We explored design principles and the key factors governing the assembly of periodic and hierarchical 3D organizations. The experimental realization of several classes of complexly organized lattices was shown and quantified by electron microscopy and x-ray scattering methods. We also investigated the information-efficient encoding of programmable interactions and the effect of information compression on the self-assembly processes. We further applied the inverse design principles, combined with selective and switchable interaction control, to establish and investigate the prescribed transformations between designed nanomaterial states. The established assembly approaches allow for the fabrication of functional nanomaterials with nano-optical, mechanical, and biochemical functions; examples of these efforts will be illustrated.