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Diamondoids-DNA nanoarchitecture: From nanomodules design to self-assembly

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Abstract

Diamondoids are one of the promising molecular building blocks (MBBs) proposed for the fabrication of a diverse range of nanostructures in molecular nanotechnology and manufacturing. The challenge is to find a route for self-assembly of these cage hydrocarbons and their application in the bottom-up synthesis. In this context, we propose a DNA-based self-assembly technique called "DNA Bridge-based Self-assembly" (DBS) to self-assemble the diamondoid molecules based upon a bottom-up strategy. The idea supporting the hypothesis is based on the well-established proofs of DNA-based self-assembly. Furthermore, the previous findings in the field of DNA nanotechnology would be inspiring to develop DBS for the construction of Diamondoid-DNA-made nanoarchitecture. The results of our computations and simulations with different molecular mechanical force fields (MM+, AMBER, BIO+, and OPLS) and different optimization algorithms (Polak-Ribiere, Fletcher-Reeves, and block-diagonal Newton-Raphson) furthermore confirm the feasibility of the formation of such hybrid nanoarchitecture.

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