Graph theoretical design strategies for self-assembling nanostructures

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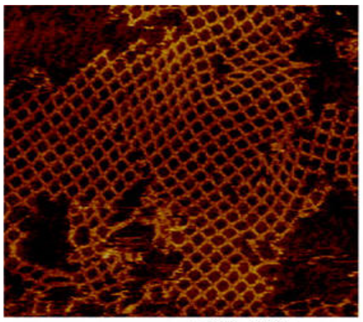
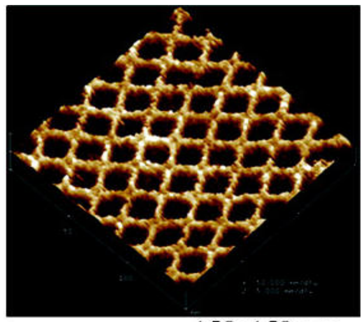


500x500 nm



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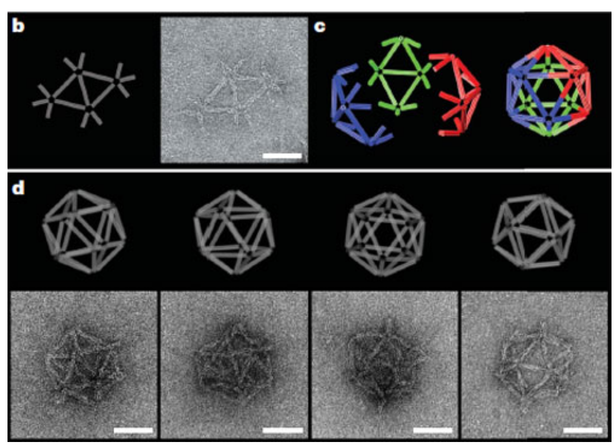
http://www.nanopicoftheday.org/2004Pics/April2004/DNAmesh

Recent advances in DNA self-assembly have resulted in nanoscale graphs: cubes, octahedrons, truncated octahedra, and even lidded boxes, as well as ultra-fine meshes. These constructs serve emergent applications in biomolecular computing, nanoelectronics, biosensors, drug delivery systems, and organic synthesis.

One construction method uses *k*-armed branched junction molecules, called *tiles*, whose arms are double strands of DNA with one strand extending beyond the other, forming a 'sticky end' at the end of the arm that can bond to any other sticky end with complementary Watson-Crick bases. A vertex of degree *k* in the target graph is formed from a *k*-armed tile, and joined sticky ends form the edges. Another construction method 'threads' a single strand of DNA through the graphical structure and then uses short 'staple' strands to fold the DNA into the desired geometric realization of the graph. A third method uses circular single strands of DNA to trace the faces of a topological embedding of the graph.

Several branches of mathematics, including topology, graph theory, geometry, are used to determine optimal design strategies for biologists producing these nanostructures. For flexible armed tiles, we define two new numerical graph invariants, the minimum number of tiles and minimum number of edge types necessary to create a given graph under three different laboratory scenarios. We determine these values for common graph classes (complete, bipartite, trees, regular, Platonic and Archimedean, etc.). For these classes of graphs, we provide either explicit descriptions of the set of tiles achieving the minimums or efficient algorithms for generating the desired set. For rigid armed tiles, we turn to the octet truss, and identify naturally occurring embedded graphs that may be efficiently constructed. Optimal threadings come from adaptations of the Chinese Postman problem, and we use genus results from topological graph theory for circular strand methods. New design strategies have led to new mathematical results, including a full generalization of duality for graphs in surfaces.



Douglas, et. al., Nature, 2009