Designed self-assembly of molecular knots, links and topological gels

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Abstract

Supramolecular constructs with complex topologies are of great interest across soft-matter physics, biology and chemistry, and hold much promise as metamaterials with unusual mechanical properties.

A particularly challenging problem is how to rationally design, and subsequently realize, these structures and the precise interlockings of their multiple molecular strands. Here we report on the combined use of theory and simulations to obtain complex supramolecular constructs via programmed self-assembly. Specifically, by controlling the geometry of the self-assembled monomers we can direct the assembly process towards "privileged", addressable topologies of molecular knots, links and extended Olympic gels.

For an actual hands-on demonstration of the designed self-assembly of "macroscopic" trefoil knots see the video at this link: www.youtube.com/watch?v=XKsuMlp2PLc

References

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