Virtual DCMIC Seminar Series 2021

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Designing molecular knots

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The self-assembly of objects with a set of desired properties is a major goal of material science and physics. A particularly challenging problem is that of self-assembling structures with a target topology. Here we show by computer simulation that one may design the geometry of string-like rigid patchy templates to promote their efficient and reproducible self-assembly into a selected repertoire of non-planar closed folds including several knots. In particular, by controlling the template geometry, we can direct the assembly process so as to strongly favour the formation of constructs tied in trefoil or pentafoil, or even of more exotic knot types. A systematic survey reveals that these "privileged", addressable topologies are rare, as they account for only a minute fraction of the simplest knot types. This knot discovery strategy has recently allowed for predicting complex target topologies [1,2,3], some of which have been realized experimentally [4,5].

References
[1] G. Polles et al. "Self-assembling knots of controlled topology by designing the geometry of patchy templates", Nature Communications, 2015
self-assembly video demonstration available at this link
https://www.youtube.com/watch?v=XKsuMlp2PLc&feature=youtu.be
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[3] M. Marenda, et al. "Discovering privileged topologies of molecular knots with self-assembling models", Nature Communications, 2018
[4] J. Danon et al. "Braiding a molecular knot with eight crossings.", Science (2017)
[5] Kim et al. "Coordination-driven self-assembly of a molecular knot comprising sixteen crossings", Angew. Chem. Int. Ed. (2018)

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