Unknotting 3-periodic entanglements of filaments and nets

Toky Andriamanalina[1,*], Myfanwy E. Evans[1], Sonia Mahmoudi[2,3]
[1]*Institute for Mathematics, University of Potsdam, Karl-Liebknecht-Str. 24-25, Potsdam-Golm, 14476, Germany*
[2]*Advanced Institute for Materials Research, Tohoku University, 2-1-1 Katahira, Aoba-ku, Sendai, 980-8577, Japan*
[3]*RIKEN iTHEMS, 2-1 Hirosawa, Wako, Saitama, 351-0198, Japan*
*email: andriamana@uni-potsdam.de

Entanglements of curves and nets can be found in various biological and chemical structures, such as in coordination polymers, in liquid crystals, or in DNA origami crystals. One example is the crystal structure of cyanamide NH_2CN, that can be regarded as the interpenetration of two enantiomorphic **srs** nets [1].

New diagrammatic descriptions of 3-periodic entanglements have been recently defined in [2]. These new diagrams are drawn out of a projection along one axis of a unit cell of a 3-periodic structure. Three projections along three non-coplanar axes constitute a *tridiagram*. It has been proven in [2] that tridiagrams fully encode ambient isotopies of 3-periodic structures, as long as the isotopies preserve the periodicity. The notion of tridiagram allowed the definition of the crossing number for 3-periodic entanglements.

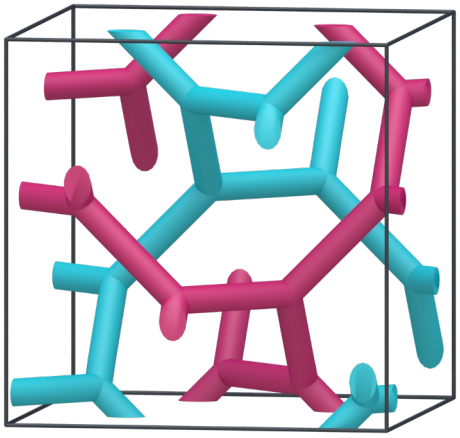

Figure 1 A unit cell of two enantiomorphic srs nets as they sit in the channels of the gyroid

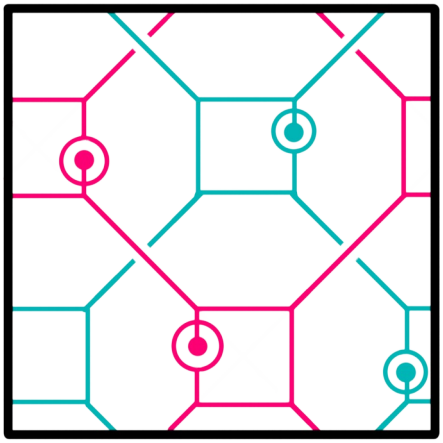

Figure 2 One diagram drawn from a projection of the unit cell of Figure 1

By using tridiagrams, we wish to extend the notion of *unknotting number* to the 3-periodic setting. We do so by listing some conditions required to transform a structure to another, whose crossings cannot be eliminated by an unknotting operation. We illustrate the practicality of this extended unknotting number on various examples of 3-periodic entanglements of curves and nets. The extended unknotting number exhibits the difference between a given embedding and the "least knotted" embedding, and the relation between them.

[1] S. Batten, R. Robson, *Angewandte Chemie International Edition*, **37**, 11 (1998).
[2] T. Andriamanalina, M. Evans, S. Mahmoudi, arXiv:2401.14254 (2024).