Symmetry-constrained ambient isotopy of piecewise-linear embeddings of decussate structures.

Michael M. J. Treacy, Michael O'Keeffe (Arizona State University)

Our study aims to identify suitable synthetic targets for molecular structures that are knotted, linked, woven, and tangled. As a rule of thumb, structures with the fewest components will be the easiest to synthesize. There will generally be two structural parts; (1) the vertices, or nodes, and (2) the linkers that connect the nodes. Usually, molecular linkers are rigid sticklike structures and cannot be relied upon to flex to accommodate the curves associated with weaves. Therefore, we seek knotted structures with the lowest vertex and stick transitivity.

Symmetry helps to minimize the transitivity. Not all symmetry groups can support knotted structures. For example, mirror planes are disfavored. Groups whose operators perform stitching actions without forcing sticks to intersect can be prolific generators of low-transitivity configurations.

Our search methods are based on a "brute-force and (mostly) ignorance" (BFI) algorithm, using our program KLiNG (Knots, Links, Nets, and Girth). As input, a judiciously chosen quotient graph, symmetry group, and cell size are provided. KLiNG randomly assigns vertex coordinates and optimizes the stick 'girth' by a gradient-descent simplex algorithm. Girth is the ratio of the shortest distance between sticks and the length of the longest stick in the model. Generally, 1 – 50 million random starts generate a histogram of girths. When there are fewer than 10 degrees of freedom, histograms present sharp peaks, which generally correspond to unique topologies of the graph (ambient isotopes). CrystalMaker, POVRAY, and Systre output files help display the structures, which can be quite beautiful.

Some nets generate infinite possibilities, and we restrict our search to the shorter 'stitching depths'. Three-dimensional weaves, links, and tangles frequently generate large numbers of ambient isotopes, making them harder to analyze.

We will present an overview of our findings so far.