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Knotted frameworks: How many distinct ways can a framework topology be realised?

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The phenomena of catenation or threading and interpenetration are found in crystal structures, from dense silicate and ice framework structures, to metal-organic frameworks [1]. One route to understanding and classifying these cases lies in the recognition of (finite and infinite) frameworks as generalisations of knots. We introduce the concept of ambient isotopy of a network and define the unknotted framework of a given topology, akin to the mathematical unknot. The definition admits some self-catenated frameworks as knot-free. Further, interpenetrating networks can also occur in distinct forms, akin to mathematical links. The approach uses the concept of equilibrium placement [2] and a number of tools recently developed to enumerate periodic frameworks via 2D hyperbolic geometry [3], accessible online as the EPINET database [4]. Explicit constructions of knotted and linked frameworks will be shown.

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Topological aspects of cell twins

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The term "cell-twin" appeared in the literature in the '70s and takes its origin from Ito's interpretation of some inorganic structures as polysynthetic repetition, via a "twinning operation", of a module corresponding to a unit cell in an archetypical structure [1]. The choice of the word "twinning" was unfortunate: the structure-building operation in Ito's polysynthetic structures acts in the point space and gives rise to a homogeneous structure; on the contrary, operations relating individuals in a twin act in the vector space and give rise to a heterogeneous edifice [2]. Apart from some adjustments in the structures of the different members built from the same module, Ito's polysynthetic structures are essentially polytypes.
Later on, cell-twins were introduced as a broader category, including Ito's polysynthetic structures, to rationalize polyarchetypal structures built by modules taken from different archetypes, with the further possibility of hosting foreign cations in the coordination polyhedra born at the boundary between two modules. When this mechanism gives rise to a series of structures whose chemistry can be expressed as a function of the type of modules and their width, it is called "tropochemical cell-twinning" [3]. Despite the modifier "cell-" the word twin remains an unfortunate choice, cell-twins being homogeneous modular structures spanning from polytypes to polysomatic series, whereas twins are heterogeneous edifices built by homogeneous individuals. To decrease possible confusion the wording "unit-cell twinning" and "crystal twinning" has been used [4].
When applicable, the concept of twinning at cell level appears useful to emphasize the topological modifications that occur at the interface between the "twinned modules". If described via this mechanism, the derivative structures appear as monoarchetypal, i.e. built up by the repetition of the same archetype module. To emphasize the specific chemical composition that occurs at the interface, i.e. the occurrence of both configurational and chemical modifications, the same structures are often described by using the formalism of the polysomatic series and considering as a different module the interface between a pair of identical modules, where the chemical change takes place. However, not all polysomatic series can be described by a unit-cell twinning mechanism.

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