

The Geometry and Topology of Crystals: From Sphere-Packing to Tiling, Nets, and Knots*

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Abstract

Crystal structures have inspired developments in geometry since the Ancient Greeks conceived of Platonic solids after observing tetrahedral, cubical and octahedral mineral forms in their local environment. The internal structure of crystals became accessible with the development of x-ray diffraction techniques just over 100 years ago, and a key step in developing this method was understanding the arrangement of atoms in the simplest crystals as close-packings of spheres. Determining a crystal structure via x-ray diffraction unavoidably requires prior models, and this has led to the intense study of sphere packing, atom-bond networks, and arrangements of polyhedra by crystallographers investigating ever more complex compounds. In the 21st century, chemists are exploring the possibilities of coordination polymers, a wide class of crystalline materials that self-assemble from metal cations and organic ligands into periodic framework materials. Longer organic ligands mean these compounds can form multi-component interwoven network structures where the “edges” are no longer constrained to join nearest-neighbour “nodes” as in simpler atom-bond networks. The challenge for geometers is to devise algorithms for enumerating relevant structures and to devise invariants that will distinguish between different modes of interweaving. This talk will survey various methods from computational geometry and topology that are currently used to describe crystalline structures and outline research directions to address some of the open questions suggested above.

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