Crystal Structure Prediction: From Topology to Geometry

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Abstract

Crystal structures are often represented as *graphs*, i.e., points (called *vertices*) connected by line segments (called *edges*) representing bonds or ligands. Atoms and molecular building blocks have particular geometries - bonds or ligands have specific lengths, and there are specific angles between them - so we might want a *geometric realization* of a graph in which edge lengths and angles between edges are specified. Tools from *geometric group theory* allow us to characterize the ensemble of all possible geometric graphs satisfying given specifications, and crystal prediction and design could benefit if this ensemble was searchable. In this talk, I will describe a demonstration program for characterizing such ensembles of (very regular) periodic graphs, and I will outline how some major stochastic algorithms currently used in crystal structure prediction might search such spaces.