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.