Crystal Structure Prediction by Vertex Removal in Euclidean Space

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Crystal structure prediction remains a major problem in computational chemistry, creating an essential barrier in the development of new materials. The problem is to find the lowest-energy crystal structures which are expected by chemists as potentially "good" ones.

The approach to crystal structure prediction that we are focusing on is to take a unit cell that has been densely packed with ions, then to remove ions from it. Our goal in the approach is to minimise the total energy with the constraint the the final charge is neutral, leaving us with a structure that may be close to a realistic structure.

The motivation for this approach from a computational perspective is twofold, first it is comprised of a simple base operation - that being the removal of an ion - which we may reason about. Secondly we can combine this approach with the opposite operation of inserting ions to reach any potential structure, allowing us to reason about the optimal arrangement for the crystal.

In this talk we will discuss this problem through the lens of graph theory, representing the structure as a set of vertices with a positive or negative charge embedded into 3-dimensional Euclidean space forming a complete graph with edges having weights corresponding to the energy between the ions in the structure. We will present a formal definition of our problem based on this input, as well as a class of functions which we may use to define the energy between ions. Finally we will conclude by showing that this problem is *NP-Complete* by a reduction from the *Clique Problem*for both the general case, and when we restrict it to the *Buckingham-Coulomb Potential* function used in chemistry.