Structural Prediction

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Abstract: More than twenty years ago, John Maddox declared that the inability to predict the structure of a crystal from its chemical composition is a "*scandal in the physical sciences*". [1] Ever since, although substantial progress has been made, structural prediction from the only chemical composition remains extremely difficult because of the complexity of the potential energy surface (PES) of a solid that is based on a large number of degrees of freedom. This clearly sets the challenge that has not to be confused with geometry optimization (or structure relaxation) which "simply" requires the knowledge of a starting geometry and a simple local minimization procedure to reach equilibrium structures with reasonable reliability. In contrast, starting from the chemical composition alone and find the minimum of the PES requires global minimization procedures that must go through efficient sampling of the N-dimension PES. To solve this global space-group problem, various algorithms have been developed in the past 10 years. These approaches are based on genetic, [2] Bayesian [3] or stochastic [4] algorithms and begin to be extensively used to discover new materials with targeted properties.

References:

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[4] D. Wales and J. Doye, J. Phys. Chem. A 101, 5111 (1997).