Predicting Crystal Structures of New High-pressure Mineral Phases

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We approached the problem of predicting crystal structures using three different methods: CMAES [1], Metadynamics [2,3] and Evolutionary Algorithms [4].

The different methods and their results for the high-pressure structures of $MgSiO_3$ and $MgCO_3$ will be presented and discussed. On the methodological side, we will focus on our implementation of an Evolutionary Algorithm based on spatial heredity and combined with local optimization. This algorithm proved to be an efficient way to tackle high dimensional problems such as crystal structure prediction and hence has a promising future in predicting, on a fully theoretical basis, new crystal structures under pressure.

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