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Building Symmetry During Crystal Structure Prediction KYLE MICHEL, CHRISTOPHER WOLVERTON, Northwestern University — Unconstrained crystal structure prediction is difficult in large cells since the number of free variables increases rapidly with the number of atoms that are included. We describe a method that builds symmetry on the fly during crystal structure prediction and uses this symmetry to reduce the dimensionality of the search space. We apply this method to Monte Carlo-based crystal structure prediction and show that simulations that build symmetry greatly outperform those that do not, both in average and fastest times to find the ground state structure.

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