

Abstract Submitted
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An Automatic Symmetry-Leveraging Approach for Solving Incomplete Many-Atom Crystal Structures BRYCE MEREDIG, CHRIS WOLVERTON, Northwestern University — We present a new first principles-based method, called a symmetry-leveraging genetic algorithm (SLGA), for fully and automatically solving large crystal structures when experimental diffraction studies do not identify all internal atomic positions. Such incomplete structural refinements may occur when crystals contain light atoms or when the characterization is performed under extreme conditions such as high pressure. We apply our method to solve the crystal structure of the promising hydrogen storage candidate magnesium imide (MgNH), which has remained a mystery for over 40 years. We also confirm *via* a fully automated procedure a recent specialized “by hand” prediction for the high-pressure phase of ammonia borane, NH_3BH_3 . The MgNH prediction, which involves 36 atoms and a notoriously complex configuration space, to the best of our knowledge represents the largest-ever crystal structure solution derived from first-principles calculations without making simplifying assumptions about atom connectivity. The 32-atom NH_3BH_3 prediction is nearly as demanding. Our approach, which takes full advantage of existing experimental information to solve for structural unknowns, has great potential for completing thousands of partially determined crystal structures.

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