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A computational–experimental approach for automated crystal structure solution

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Crystal structure solution from diffraction experiments is one of the most fundamental tasks in materials science, chemistry, physics and geology. Unfortunately, numerous factors render this process labour intensive and error prone. Experimental conditions, such as high pressure or structural metastability, often complicate characterization. Furthermore, many materials of great modern interest, such as batteries and hydrogen storage media, contain light elements such as Li and H that only weakly scatter X-rays. Finally, structural refinements generally require significant human input and intuition, as they rely on good initial guesses for the target structure. To address these many challenges, we demonstrate a new hybrid approach, first-principles-assisted structure solution (FPASS), which combines experimental diffraction data, statistical symmetry information and first-principles-based algorithmic optimization to automatically solve crystal structures. We demonstrate the broad utility of FPASS to clarify four important crystal structure debates: the hydrogen storage candidates MgNH and NH3BH3; Li2O2, relevant to Li–air batteries; and high-pressure silane, SiH4.

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