Decoding crystal structures: a deep learning approach to the phase problem

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Our research builds upon and extends the work presented in [1], offering a novel neural network approach to solve the crystallographic phase problem with a resolution of just 2 Å. By synthesizing millions of artificial structures along with their corresponding diffraction data, we have used an extensive training dataset for the neural network. This pioneering approach enables ab initio phasing with only 10%to 20% of the data conventionally needed, thereby challenging the prevailing belief that atomic resolution is essential for structural solutions. The neural network adeptly handles data within standard centrosymmetric space groups and moderate unit cell dimensions, highlighting its potential to broaden the applicability of neural networks for the phase problem. This method holds significant promise for enhancing the structural determination of weakly-scattering crystals, such as metal-organic frameworks and nanometer-scale materials.

[1] Larsen A S, Rekis T and Madsen A Ø 2024 *Science* **385** 522–528