Data-Driven Methods for Acceleration of Crystal Structure Prediction

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Crystal structures are key to deeply understanding the various physical and chemical properties of condensed matter, and they also form the basis for theoretical materials modeling, simulations and discovery. Theoretical crystal structure prediction of materials, given only their chemical compositions, is crucially important. However, this task is extremely challenging as it involves identifying a vast number of energy minima on the lattice energy surface.

In this report, I will first provide a brief introduction to the CALYPSO structure prediction method. Following that, I will detail our recent advancements in accelerating structure prediction through data-driven approaches, such as machine learning potentials and generative models. Through several benchmark and practical applications, we demonstrate that data-driven approaches are heralding a new era in crystal structure prediction.