Oral presentation

A seventh blind test of crystal structure prediction methods

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Crystal Structure Prediction (CSP) – generating and ranking plausible crystal structures from a chemical diagram – is a rapidly evolving field, offering a diverse set of methods for predicting polymorphism of molecular crystals, directly informing the solid-form design process.

Since 1999 the CSP blind tests, a community initiative coordinated by the Cambridge Crystallographic Data Centre (CCDC), have provided CSP methods in development with an opportunity to validate and benchmark methodologies against unpublished data [1-6]. Here we present key results from the recent seventh blind test [7-8] which involved participation from 142 researchers from 28 groups in both academia and industry. CSP is on the precipice of widescale accessibility and affordability with the increasing efficiency of methods for exploring structural space and ranking the stabilities of large numbers of crystal structures.

These results demonstrate the tremendous improvement in predictive capabilities of CSP methods while highlighting urgent challenges for the community to address. This talk provides an overview of the state of the art in CSP for those less familiar with the field, understanding applications and limitations of methods.

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