What Have We Learned From the 7th Blind Test of Crystal Structure Prediction? – Triumphs, Challenges, and Insights

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Predicting the experimentally accessible crystal structures of a molecular material is one of the fundamental challenges of solid-state science. Since 1999 the Crystal Structure Prediction (CSP) blind tests, organised by the Cambridge Crystallographic Data Centre (CCDC), have provided an unbiased assessment of state-of-the-art methods from CSP, with subsequent publications capturing the developments made over the years and providing readers with an overview of the methodologies available and in-development. To date, 7 blind tests have been carried out with the most recent ending in June 2022.

In this talk we will present the major developments and remaining challenges facing CSP methods as evidenced by the outcomes of the 7th blind test, and explore the structural-energetic insights gained from analysis and graphical visualisation of crystal structure landscapes submitted.