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EuCompChem2025 – Jennie Martin – Oral :Re-Using Computational Data: Fast Molecular Crystal Structure Prediction by Analogy to Prior Predicted Landscapes

This talk discusses our work to develop a fast approach to organic molecular crystal structure prediction (CSP) by using previously predicted CSP landscapes of similar molecules to guide sampling within our structure searches. We discuss the method developed, initial results found, and the promise of the approach considering the 'big data' direction of the CSP field[1]. We will also touch upon potential applications of the approach to the discovery of porous materials.

With the growth of the materials discovery field, large amounts of structure prediction data are being generated – one recent study calculated the CSP landscapes of over 1000 small molecules[1]– and the impact of that data can be extended by exploring effective ways for its re-use when studying new molecules. One application, not reliant upon machine-learning, may be in using existing prediction data to aid further CSP, by use of analogy in the generation of trial crystal structures.

We discuss our approach to quickly generate CSP landscapes of target molecules, by generation and optimisation of analogues (Figure 1) of previously predicted crystal structures of similar molecules. The method demonstrates a proof of concept for how analogy-based CSP approaches used more commonly in the inorganic CSP community can also be used for molecular systems and could utilise previous computations – avoiding a reliance upon experimental structure data.

Tested on a variety of small organic systems, the method has shown promise in predicting the crucial low-energy regions of CSP landscapes with greatly reduced sampling compared to quasi-random approaches. Initial findings suggest a similarity of the CSP landscapes of similar molecules and demonstrate potential broad applicability of the approach.

The talk will introduce our work including generation of reasonable crystal structure analogues, the utility and efficiency of the approach in structure prediction, potential applications in materials discovery, and our thoughts on where the method can take advantage of the increasing availability of computational data.

1- C. Taylor, P. Butler and G. Day, Faraday Discuss., 2025, 256, 434–458.

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