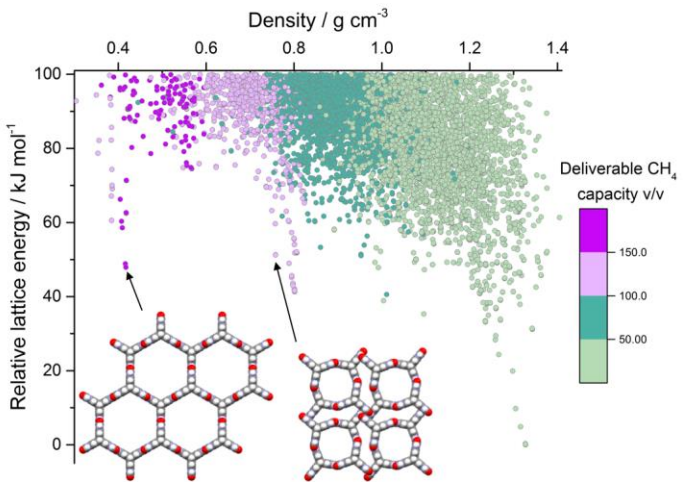
Case Study: N8 HPC and the University of Liverpool

Functional Materials Discovery



Testimonial

"The N8 HPC facilities, together with the local University of Liverpool ones, shared the whole workload of over 1,000,000 serial jobs. The particular things we appreciate about N8 HPC include its impressive computing capability and capacity, simple and straightforward application procedure for access, and the extremely accessible and helpful local support team."

Dr Linjiang Chen - Cooper Group, University of Liverpool.

Project

A fundamental goal in materials research is to design new functional solids. This is guided by calculations and done at the very beginning of a material discovery workflow. Molecular crystals are particularly difficult to design as they do not assemble following simple, intuitive rules. Their structure results from the balance of many weak interactions unlike the strong and predictable bonding patterns found in metal–organic frameworks and covalent organic frameworks. Predictive strategies that do not rely on intuitive bonding rules, such as crystal structure prediction methods, are needed to enumerate potential arrangements of molecules. It is a major challenge, however, to identify crystal structures that can be realized in the laboratory.

The discovery and design of functional molecular crystals requires computation of both the material property of interest and the material's stability with respect to alternative atomic configurations. To predict, select, and then synthesize exciting new materials (which has been done to improve Li-Ion batteries), a simple, digestible description of the probable structure–function space is much more desirable than the potential space, which are often astronomically large. We took on this challenge by combining computational crystal structure prediction and property prediction to build energy–structure–function (ESF) maps. An ESF map is a collection of predicted structures and their properties, representing the possible material properties associated with the molecule.

Partners

Professor Andrew Cooper – Cooper Group, University of Liverpool

Professor Graeme Day– University of Southampton.

Dr Linjiang Chen– Cooper Group, University of Liverpool.

Impact

This work heavily relied on the intensive uses of local, regional, and national HPC facilities. N8 HPC was of paramount importance in enabling us to manage the heavy workload of structure and property predictions efficiently. This provided our experimental colleagues with 'treasure maps' so that they could better focus their synthetic efforts (where to look) and target specific applications for different materials (what to look for). The N8 HPC facilities, together with local HPC facilities, shared the whole workload of materials property calculations, which amounted to over 1,000,000 serial jobs. The things we appreciate greatly about N8 HPC include its impressive computing capability and capacity, simple and straightforward application procedure for access, and the extremely accessible and helpful local support team.

During the revision of the paper, we were working toward a tight deadline, with a large number of simulations remaining to be done. It was extremely helpful that we were granted access to the N8 HPC facilities within days of application and also that the throughput on the cluster was really impressive.

Success

Our research essentially described a new strategy for finding functional organic crystals using ESF maps. Crucially, the method assumes no underlying topology or structural blueprint, and hence it can be applied to new, hypothetical molecules that have no precedent, unlocking the creativity of synthetic chemists. Furthermore, this research was recently published in a paper in *Nature* (543, 657-664, 2017) where all the data is open-access. It won't be too hard to envisage that some of the predicted structures may be realized by other researchers or some more sophisticated analyses of these ESF maps will reveal richer information currently going unnoticed.

N8 HIGH PERFORMANCE COMPUTING

UNIVERSITY OF LIVERPOOL