

Accelerating the development of unique materials using computer modelling

Funded by the Science and Technology Facilities Council's (STFC) Bridging for Innovators programme, the Hartree Centre worked with material specialists Lucideon to accelerate the development of novel ceramics.

Challenge

One of the biggest challenges in material discovery is knowing where to start. Lucideon's focus was on producing high entropy ceramics, novel materials composed of five or more different types of cations or anions. While such materials are relatively new to industries, they are now gaining ground due to their usefulness in a broad range of application areas.

The production of a high entropy ceramic requires selecting groups of five or six elements out of a much larger pool of available components. Lucideon began with fifteen possible elements which offered more than 8000 possibilities, highlighting the vast scale of the materials search space. It is a monumental task to explore these possibilities and even after reducing the initial selection to a shortlist the team were left with over 5000 candidates.

Solution

Through the Bridging for Innovators programme, Lucideon combined many years of developing ceramic systems with the STFC Hartree Centre's expertise in data science, computational materials science and atomistic modelling. This collaboration built upon advanced computer modelling and data analysis techniques

and began to solve the challenge that comes with exploring unique materials.

Lucideon used simulation as a compass, to guide and help pin-point a region of composition space prior to experimentation. The Hartree Centre developed an atomistic modelling methodology in the sweet spot between precision and scalability that enabled them to computationally estimate the properties of all 5000+ candidates, which would not have been possible at higher fidelity without investing infinite time and budget. After this step, Lucideon narrowed down the 5000+ candidates to five that were then synthesized in the lab.

Benefits

The main benefit of this collaboration was the exploration of unique materials that did not exist before, supporting the scale-up for a range of urgent applications across multiple industries such as the energy sector and aerospace.

One significant technical outcome was that the Hartree Centre's computational predictions were shown to be accurate when compared with Lucideon's experimental data, demonstrating the model's usefulness in future applications.

Through this project, Lucideon were able to marry experimental and computational workflows to de-risk material discovery and greatly increase the speed of identifying desirable candidates in a complex and vast search space, thus accelerating the product development cycle of novel ceramics.

"Developing new materials to meet emerging needs can take many years, even decades, to achieve with no guarantee of success. What the B4I programme allowed us to do was apply our experience at Lucideon in collaboration with experts at the STFC Hartree Centre leading to a significant reduction in the time it has historically taken to identify attractive materials for a specific application. The outstanding results demonstrated that it is possible to develop custom materials with higher confidence and lower risk when the two groups attack a problem from multiple angles and perspectives."

Richard Padbury
Senior Consultant, Lucideon

About us

Science and Technology Facilities Council offers entrepreneurs, start-ups, SMEs and corporates the facilities, environment and people needed to de-risk innovation and accelerate business growth.

Through access to large-scale science facilities, complementary technologies and IP, and a flourishing network of science and industry experts, companies can create and transform products.

Bridging for Innovators provides funding for companies to utilise STFC facilities and expertise to fast-track solutions to industrial challenges and boost productivity.