



Accelerating materials discovery

Funded by the Science and Technology Facilities Council's (STFC) Commercial Pump Priming Fund, the Hartree Centre developed Hartree-MaDE, a new computational tool for materials discovery.

Challenge

Computational materials discovery involves searching vast material spaces for potential candidates that have the optimal combination of suitable properties for target applications. High fidelity predictions are required to make meaningful predictions so navigating a material space containing tens or hundreds of thousands of materials is a significant challenge. A tool that can help navigate through a maze of candidate materials will help accelerate the discovery process.

Approach

The Hartree Centre's Materials Discovery Engine (Hartree-MaDE) is a tool that simplifies and automates the process of materials discovery. Its main focus is on alloy discovery - particularly substitutional high entropy alloys – but the tool can model all hard materials that exhibit crystalline order, including solid ordered phases of polymers. It relies on so-called descriptors to predict the stability of alloys from the mechanical properties of the component materials, which are predicted at high fidelity using state-of-the-art density functional theory. Observable properties of the alloys are similarly predicted from those of the component materials, via carefully chosen averaging schemes. The only user input required is the structure and composition of the component materials. Hartree-MaDE then automatically builds the database of every possible substitutional alloy that can be engineered from combinations of the base materials, allowing users to go forward and quickly identify the best candidate materials for their target application.

Benefits

Using Hartree-MaDE to screen an initial set of materials de-risks and accelerates materials discovery while significantly reducing development costs. Businesses can use the software to supply them with candidate materials without the need for expensive trial and error procedures in the lab. By predicting a broad range of both thermal and mechanical properties, Hartree-MaDE can help businesses identify and develop new hard materials. Future versions of the tool will include an active learning AI algorithm that will further enhance fidelity and continue to accelerate materials discovery.

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Working with The Hartree Centre enabled us to efficiently explore an extremely complex area of ceramic material discovery for a niche application where currently available options are far from ideal.

Richard White
Lucideon

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The technology underpinning the Hartree-MaDE engine enabled us to pin-point viable options from 5000+ potential candidates for a materials based solution. This work opened my eyes to the power of computational methods for material solutions.

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Richard White, Principal Consultant - Materials
Lucideon

At a glance

- New tool for simplifying and automating new materials discovery
- De-risks discovery and reduces development costs
- No need for expensive trial and error procedures
- Builds a database of every possible substitutional alloy from combinations of base materials
- Quickly identifies the best candidate materials for your application

Who we are

- 70+ computational scientists and technologists
- World-leading supercomputing and AI infrastructure
- Bespoke small teams built around your project
- Tailored business development support
- Access to our network of industry, academic and technology partners

What we do

- Boost productivity and enhance innovation for industry
- Big data analytics and artificial intelligence (AI)
- High performance computing and quantum simulation
- Training and skills development
- Insights into future technologies



Credit: STFC Hartree Centre

Our impact on UK industry and society

The Hartree Centre was created by UK Government to help businesses and public sector organisations accelerate the adoption of high performance computing (HPC), big data analytics and artificial intelligence (AI) technologies. We play a key role in realising UK Government's Industrial Strategy by stimulating applied digital research and innovation, creating value for the organisations we work with and generating economic and societal impact for the UK.

The Science and Technology Facilities Council (STFC) Hartree Centre is part of UK Research and Innovation.