Researchers based at the STFC Hartree® Centre worked with Johnson Matthey, using computational techniques to automate and accelerate the process of identifying properties of novel chemical formulations.

**Challenge**

Chemical formulation is at the heart of many manufacturing processes. It is critical in areas as diverse as medication, personal care products and engine oils. Typically, formulation research is carried out experimentally in a laboratory. Johnson Matthey were looking for a way to automatically predict the properties of novel formulations, generating strong reproducible insights into product development. These computational tools would enable digital pre-screening of novel formulations, guiding the decision making behind which new formulations should be prioritised for expensive laboratory testing.

**Approach**

Researchers applied state of the art computational modelling techniques to uncover processes and interactions occurring at the molecular level in much more detail. The team developed computational tools capable of fully automating complex experimental methodologies with the ability to predict a new formulation’s critical properties, such as phase behaviour and rheology. These complex methods are fully automated to ensure they are reusable and accessible for non-expert users. The project has offered new insights, allowing the detailed visualisation of chemical structures and interactions formed in novel chemical formulations.

**Benefits**

These tools – Developed as part of the Innovation Return on Research (IROR) programme, a collaboration between STFC and IBM Research – use computational techniques to investigate the critical properties of novel formulations before having to invest time and valuable physical resources into producing an unproven formulation. This work has the potential for widespread impact, allowing formulators to operate more efficiently with less waste and focusing resources on the most probable formulation from the outset. The automation of these tools and processes will enable non-expert users to access high performance computing resources.

> "Working in collaboration with the Hartree Centre is enabling us to explore new digitisation methods, which could change the way we formulate in the future to ultimately save us valuable time and money."

— Misbah Sarwar
Johnson Matthey

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At a glance

- Investigating whether computation can provide useful insights and predictions for polymeric formulations
- Saves valuable time and resources associated with expensive laboratory testing upfront for unproven formulations
- Developed computational tools to fully automate complex simulations and analysis
- Boosting efficiency and reducing waste by focusing resources on the most probable formulations from the outset

Who we are

- 60+ 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 emerging technologies

Our impact on UK industry and society

The Hartree Centre was created by UK Government to transform industry by accelerating 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.

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