

# Enhancing packaging R&D with clay-polymer modelling



Hartree Centre  
Science & Technology Facilities Council



The STFC Hartree Centre has helped Sun Chemical, a leading supplier of printing inks, pigments and coatings, realise the value of clay polymer-modelling to improve its packaging R&D methods.

## Challenge

Sun Chemical is recognised as a leading source of innovation to various industries including publication and packaging. The company creates solutions that improve productivity, create new revenue opportunities for customers, and contribute to a more sustainable future. As such it is continually looking for innovative ways to advance its products and services. The primary function of packaging is to protect its contents, for example, keeping food fresh by separating it from external factors such as moisture and oxygen. Though perhaps not an obvious choice, clay particles show promise as an effective and inexpensive candidate to use in coatings to improve this barrier. For Sun Chemical to implement new packaging solutions, they require efficient and cost effective ways to test potential new materials.

## Solution

The Hartree Centre, alongside partners Durham University and University College London (UCL), conducted a pilot study with their technical capabilities to introduce Sun Chemical to computational modelling as a method of testing new materials. The project, part-funded by METRC, allowed researchers to observe how clay particles disperse in a solvent-polymer mixture at the molecular level. Researchers designed new dispersions or packaging candidates virtually and were able to accurately predict how they would behave before advancing to real-life testing.

## Benefits

With computational chemistry models, scientists can observe what happens to individual molecules. This means they gain an insight into not only the “what” but also the “how” and “why” of a process. Along with providing more useful results, this method is much more time and cost effective, as it reduces the need for physical prototyping and experiments. Introducing savings to just 5% of the global food barrier packaging market with an environmentally friendly clay-polymer technology would be worth around £150m of new business to Sun Chemical. The company now has the potential to utilise the method in future R&D.

*“With this kind of advanced modelling, you can watch what happens on an atomistic level so you really understand the reasons behind it, rather than just seeing the end result. In a real-life experiment, you see whether it works, but you don’t see why. Sun Chemical now has the knowledge to benefit from these techniques in future R&D.”*

– Sebastian Metz, Computational Chemist, STFC

## Work with us

We collaborate with industrial clients and research partners on projects that create insights and value using high performance computing, big data analytics, simulation and modelling.

By combining our world-class facilities with access to our specialists and computational scientists, we can enable your organisation to produce better outcomes, products and services more quickly and cost-effectively than through conventional R&D workflows.

With our partners we are developing the next generation of supercomputing architectures and software, combining existing best practice with innovation to deliver faster, cooler and more sustainable solutions capable of meeting the challenges of data intensive computing.

## For more information:

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