Science and Technology Facilities Council

Scientific Computing

Addressing Industry Challenges with Materials Modelling

A major challenge we face today is to understand the effects of materials used in every day products and services, from plastics in food to storage containers for nuclear waste.

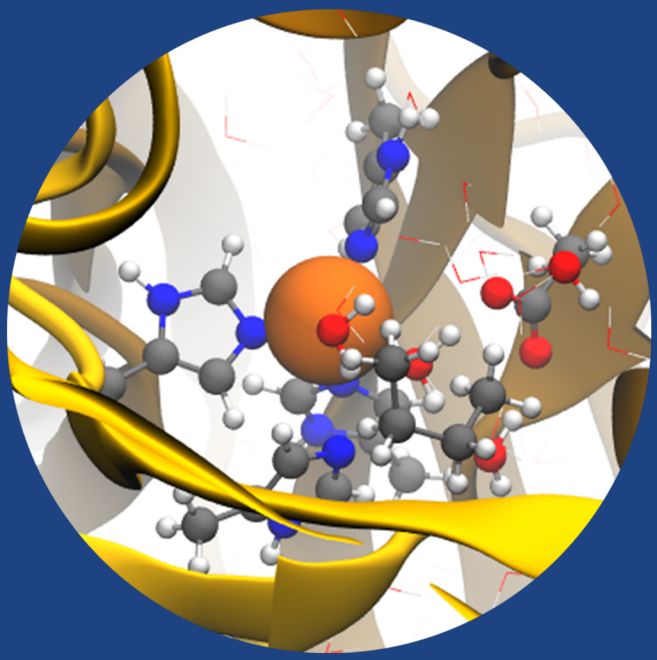
Computational scientists at STFC Scientific Computing are exploring these challenges by developing tools that can help a wide variety of researchers and industries.

The field of materials modelling relies on computational software to accurately calculate the physical properties of molecules and simulate materials behaviour under different conditions. Such tools can be used in a wide variety of industries to provide companies with the ability to test prospective materials solutions before manufacturing, and provide cost effective methods for virtual screening of the changes in their molecular structure and behavior during processing.

Scientists from Scientific Computing's Computational Chemistry Group at Daresbury Laboratory have developed simulation products to support academia and industry worldwide, including computational methods for studying complex chemical systems ranging from materials used in industrial scale chemical production to bacterial proteins.

The expertise within this group also ensures that the software can run efficiently on a wide variety of computer platforms, from a desktop PC to massively parallel supercomputers.

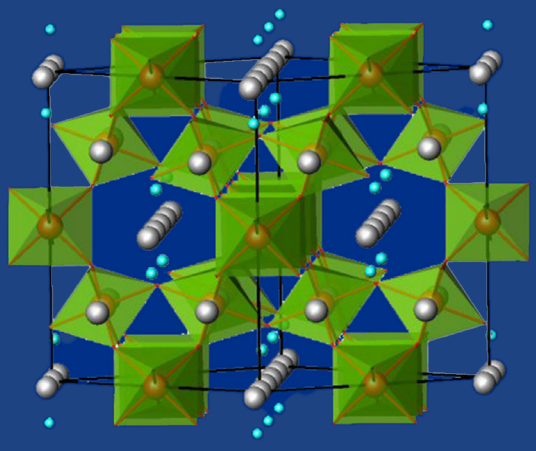
As well as modelling the composition and behaviour of materials, the group can streamline workflows and poivde data-handling solutions ensuring that researchers can concentrate on their studies rather than spending time on computing requirements.



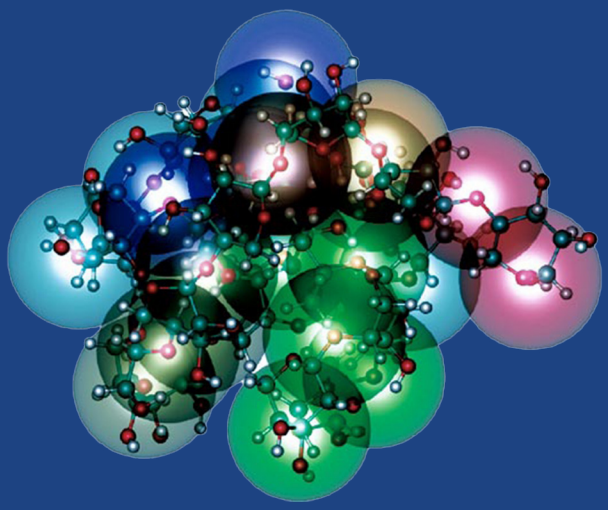
A catalytic copper centre in a nitrite reductase enzyme for a hybrid multiscale modelling calculation with ChemShell. (Credit: Thomas Keal)

The software is already being used in a variety of different industries and applications, including:

- Developing a tool designed to simulate the effects of radiation damage in materials, which has become incredibly useful in experimental and theoretical research into the ageing of materials exposed to radiation. The software can simulate how materials age through time in various environments, and temperature and pressure ranges
- Designing and developing new pharmaceutical products, or improving existing products
- Testing the damage and micro-structural changes of spacecraft surfaces when they collide with microscopic meteor particles in space, an experiment that would be impossible to perform on Earth
- Investigating why plastic particles penetrate into food, how they can be used in cosmetic products, and exploring the effects they may have on cell membranes either in the food or in the human body
- Investigating the structure of bones and teeth.



Pyrochlore (Credit: Ilian Todorov)



Off-lattice representation of oligosaccharide superimposed on corresponding atomic configuration (Credit Dmytro Antypov)

For more information and to gain access to the suite of materials modelling software please visit our website at:

www.scd.stfc.ac.uk/Pages/Materials-Modelling-Software.aspx

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