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Automated computer workflow opens up opportunities for a greener future

Research fuelled by STFC Scientific Computing's new 'Automated Potential Development' (APD) computer workflow has already led to the identification of a new class of thermoelectrics called 'incipient ionic conductors', which can help reduce climate change by converting heat into electricity, reducing reliance on fossil fuels and decreasing greenhouse gas emissions.

Now it is helping to open up new horizons for inorganic materials science—allowing research into the properties of materials on the atomic scale. It enables a move to embrace the benefits of machine learning and computer modelling as complementary tools for experiments within the ISIS Neutron and Muon Source and other large-scale high-energy particle accelerators. This in turn allows research at a much larger scale and over longer timescales.

The Challenge

Currently, experimentalists in materials science are constrained. They have to work with a simulation cell which limits the size of the 'box' where the atoms are under scrutiny. In many cases this restricts research to instances where only a small number of atoms can be feasibly modelled using Density Functional Theory (DFT—a method used in chemistry and physics to calculate the electronic structure of atoms, molecules and solids).

However, if the research involves scrutinising behaviour of atoms for longer timescales or at a larger scale, then DFT would not be the most suitable method to give accurate results.

The real-world experiments currently being undertaken give researchers a graph which shows diffusion, but the results don't show the atoms moving, **where** they are moving or **how** they are moving.

Developing specialist computer models for researchers within the ISIS community would normally not be possible due to constraints around funding, and because bespoke models would need to be developed for each experiment.

Even if the skills were available, developing the models would typically take three months or more and involve computational modelling experts working with the experimentalists to set up and run the computer aspects of the research.

> **"There are simply not enough computer experts in the world to help every experimentalist, which is why we've developed APD."**
>
> **Dr Andrew Duff**
> Senior Computational Materials Scientist, STFC Scientific Computing.

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Our Approach

In his role as Project Investigator and lead coder, Andrew Duff has developed the Automated Potential Development workflow. It takes data from the results of experiments based on Density Functional Theory and trains models using APD to allow researchers and beam-line scientists to magnify the size of the cell, and to research longer and bigger timescales. This can be used to run simulations to see how the atoms move.

A 'potential' is a highly sophisticated computer model.

> **"Even among computational modellers only a small fraction specialise in developing potentials. The field of automatically generating potentials using machine learning is a new and exciting area of computing."**
>
> **Dr Andrew Duff**
> Senior Computational Materials Scientist, STFC Scientific Computing.

Initially the ISIS Neutron and Muon Source team used the APD in a collaboration with the University of Reading to investigate tetrahedrite, a type of mineral with promise for converting waste heat back into electricity. Such 'thermoelectric' materials have the potential to reduce energy emissions and help fulfil net-zero targets by providing a sustainable energy resource.

For the tetrahedrite research, the initial experiment at ISIS yielded unexpected results. They showed a 'QENS signal' (Quasi-Elastic Neutron Scattering), implying atoms could move freely in the solid, contradicting the previously accepted view that atoms in tetrahedrite would remain immobile.

APD not only corroborated this QENS signal but also provided a crucial explanation: while copper atoms do move within the solid, they are prevented from moving too far as they spend most of their time trapped in cages formed from the crystal structure.

Benefits

This research led to the identification of a new class of thermoelectrics called ‘incipient ionic conductors’, offering the possibility of high efficiency without the usual wear, and opening up a new avenue in the search for thermoelectric materials.

In more recent work on ZrW_2O_8 (Zirconium Tungstate Oxide), APD has been used to develop models predicting the dynamic coherent structure factor—an observable also measured at ISIS.

This work focuses on ZrW_2O_8’s unusual property of negative thermal expansion, which has potential applications in precision engineering and temperature-stable materials. For instance, it might be used for advanced thermal coatings in aircraft, for precision and stability in medical implants, or as a reliable material for electronic components.

> **“APD has allowed us to interpret experimental results and elucidate the mechanisms behind this behaviour.”**
>
> **Dr Russel Ewings**
> ISIS Neutron and Muon Source.

The APD has also been applied to LLZO (Lithium lanthanum zirconium oxide), a promising battery material, and has given insights into diffusion mechanisms that enhance its energy storage potential. These materials are currently of great scientific interest due to their potential applications in electric vehicles.

> **“By making cutting-edge machine-learning based MD simulations accessible to neutron experimentalists, APD promises to transform our understanding of a broad range of phenomena in the solid state.”**
>
> **Dr Gøran Nilsen**
> ISIS, Principal Investigator on the LLZO project.

The APD is also being used by the STFC Hartree Centre to investigate how material composition affects the temperature-dependent strength and stress-strain relations in multi-component crystals.

These are all significant advancements made possible by the APD workflow, highlighting its impact on materials science and its potential to contribute to a greener future.

More Information

The APD is fully automated and with a ‘front end’ which researchers without specialist computing skills can use.

The Alpha release of APD is already available and is open source, available to any user. Version 1 should be available later in 2025.

Although the APD was designed for the ISIS facility researchers, it will be useful for researchers in both academia and industry, in any area of materials science where a potential would be useful to further understanding of atoms and their positions.

It is particularly effective in modelling the interactions between atoms, making it valuable for studying materials such as steels, advanced alloys, and high-entropy alloys. It is especially useful when exploring material properties like strength, stress-strain responses, and more intricate microstructures.

Andrew Duff’s work was funded by a grant from the Ada Lovelace Centre to raise the impact of Facilities’ science and help experimentalists to do complementary modelling and to help give their experimental studies a higher impact.

Gøran Nilsen and Andrew Duff are part of an international collaboration that has secured a grant from the Norwegian Research Council to further develop the Automated Potential Development workflow to allow researchers to use it to analyse LLZO and other materials relevant to battery technology.

Further Reading

Can thermoelectric tetrahedrite stand the heat?

Beyond rattling: tetrahedrites as incipient ionic conductors

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