PhonIon: Modelling ultrafast THz pump-X-ray probe spectroscopies for ion dynamics in batteries

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Hi, my name is Raj Pandya and I'm an Assistant Professor in Physical Chemistry at the University of Warwick. Today I'd like to introduce you to our project Phonelon for the 2025 HetSys cohort.

This is a project that's going to be done with my colleague Reinhard Maurer in Chemistry and Nick Hine in Physics, and it's going to be all around modelling ultra fast terahertz and X-ray pump probe experiments to be able to follow iron and electron dynamics inside lithium-ion battery materials.

So as many of you will be aware, lithium-ion batteries are revolutionising the world we live in. And at their core they're driven by the motion of lithium ions and by electrons. How those lithium ions and electrons move through our battery materials and through our lattices really governs how efficient the battery material will behave.

But unfortunately, understanding this is quite challenging. One of the tools that scientists have developed over the last 10 and 20 years are ultra fast X-ray experiments. So this is where we take short bursts of X-ray light and use that to watch inside our materials the challenges, these X-ray experiments are really hard to interpret.

The data looks very much like just a random stream of information, but in it is hidden the key information to unlocking how the battery materials are operating, how they're being efficient and ultimately to be able to drive new battery technologies.

So what we're going to be doing in this project is unlocking the new software tools and new modelling methods to be able to understand these ultra fast X-ray experiments in batteries and really unlock this nascent information about electron and ion dynamics inside our battery materials.

We're going to be focusing on modelling two types of XFEL or ultra-fast X-ray experiments. One is called a terahertz pump X-ray probe experiment where we use one laser pulse to drive the ion motion and another to watch it and we're going to be able to see using particularly machine learning methods, how we can actually understand how those ion dynamics are moving from the data in those experiments.

And then there's going to be a second type of experiment called X-ray photon correlation spectroscopy. This is an experiment which where we can understand lattice fluctuations in our system.

And so we get lots of very, very noisy data. The question is going to be how to turn that noisy information into useful information about our battery dynamics and ultimately unlock the key recipes and the clean ingredients inside our battery systems.

In this project, what you're going to learn is a variety of advanced computational methods, many of which are going to be focused around machine learning. You're going to get a great understanding of quantum dynamics and using quantum dynamics to be able to understand lithium-ion battery materials for the first time.

And ultimately, you're going to be able to derive and design new X-ray scattering geometries that will be used by thousands of scientists around the world. And those software and tools will be used by others to be able to generate new information on battery systems.

If you'd like to chat with me, feel free to get in touch via e-mail or through the Hetsys website.

Thank you.