Coding, Collaborating and Communicating to keep energy materials discovery and development flowing

CoSeC
Computational Science Centre for Research Communities

Angela Harper, a 3rd year PhD student in the Physics Department at the University of Cambridge, wrote the joint, 3rd-placed winning entry for the 2021 CoSeC Impact Award. Angela's research brings the computational expertise of theoretical physicists using atomistic modelling methods and software developed within the Collaborative Computational Project in Electronic Structure (CCP9), to not only experimental chemists, but to the wider community. This accelerates both discovery and identification of industrially relevant and new materials using computational methods, thereby reducing the costs, energy and time involved in conducting large-scale experimental studies.

Background

Discovering new materials through experimental pipelines is a time-consuming and expensive process, involving large amounts of trial-and-error and expensive experimental equipment.

Many devices at the forefront of research fall into the category 'solid state' e.g. battery materials, and an increasing number of these are also classified as 'amorphous', which proves particularly challenging to experimental characterization.

Computational research of solid state materials originated with crystalline materials where the atomic structure forms a regular, repeating pattern that is readily identifiable experimentally. These structures are characterizable through first principles (i.e. from fundamental concepts) computational methods such as density functional theory (DFT). With its foundations in quantum mechanics, DFT calculates the positions of atoms and the electronic structure of a material.

In contrast, amorphous materials are non-crystalline and their structures are difficult to predict computationally and to characterize experimentally. A specific example is the structure at interfaces of solid state battery materials.

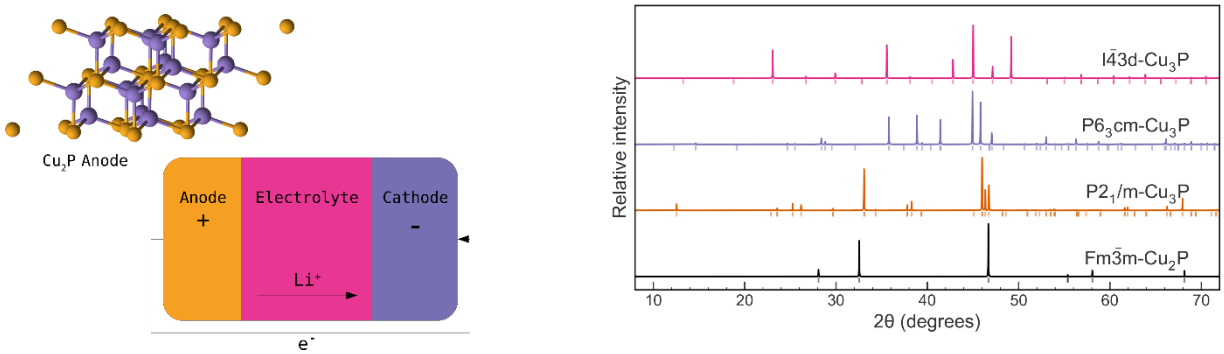
Challenges

A major challenge in materials sciences is **characterizing the structures of amorphous materials.** Access to large-scale characterization facilities e.g., synchrotrons is competitive and often requires experimental evidence, but for new and difficult-to-characterize materials this is often lacking. One solution lies in predictive, computational data, which leads to a second challenge: the **data's availability and accessibility**. Even where available, it can remain invisible to experimental researchers due to a lack of awareness of, and/or access to, both the relevant journals and databases storing the data. The third major challenge is the **diversity of research groups**, from personal identity to research disciplines and methods. Diverse perspectives lead to innovative progress, but can be difficult to achieve due to the silo effect of specializing in one discipline, e.g. as an experimentalist or a theorist, and the inevitable communication barriers that exist between them.

Angela's role in addressing the challenges

Angela used computational methods to accelerate both discovery and identification of industrially relevant materials. She developed a structure prediction workflow involving ab initio random structure searching (AIRSS), structural prototyping, and a genetic algorithm, to discover a novel copper phosphide anode material for lithium-ion batteries. Addressing accessibility, Angela compiled the data from the structure prediction into an open-source Jupyter Notebook[1]. This format allows direct downloads and has already yielded experimental interest in these industrially relevant materials. Angela also developed a method – involving two CoSeC-supported codes[2] – for calculating spectroscopic signatures of amorphous phases[3].

Finally, Angela actively sought to promote diversity and communication across scientific communities by speaking at events about their research and experience as a woman in science. These include: as a Tutorial leader for a DFT code workshop; presenting the importance of studying Li-ion batteries at the Churchill College Graduate Talk series to an audience across disciplines; and as a speaker at the Cavendish Inspiring Womxn seminar series.



Left: predicted model of copper-phosphide anode and right: its computationally predicted powder x-ray diffraction (PXRD) pattern. Spectra reused with permission from ACS, https://pubs.acs.org/doi/full/10.1021/acs.chemmater.0c02054

CoSeC's Impact

> "Being part of the CCP9 community gives me the support and platform I need to connect and collaborate with other researchers. For example, through CCP9-organised workshops I can promote open-access research, work closely with experimentalists and use scientific outreach to engage with a wide range of communities"
>
> Angela Harper

CCP9 is the Collaborative Computational Project for the Study of the Electronic Structure of Condensed Matter, providing a network connecting UK research groups in electronic structure, facilitating UK participation in the larger European Psi-k Network, and supporting a number of cutting-edge computational codes.

www.cosec.stfc.ac.uk

@CoSeC_community

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Further information: https://mybinder.org/v2/gh/harpaf13/data.copper-phosphides/master?filepath=CuP_results.ipynb; [2]Castep and Soprano; [3] This lead to the characterization of a ubiquitous industrial coating material, amorphous alumina, via nuclear magnetic resonance (NMR) and X-ray absorption spectroscopy (XAS); these spectra are the first ab initio spectra on amorphous materials to date.

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