UNIVERSITY OF BIRMINGHAM

School of Metallurgy and Materials

PhD studentship in the Computational Structure Prediction of Energy Materials

A 3-year UK/EU PhD student-ship is available in the group of Dr Andrew J. Morris who has recently relocated to the School of Metallurgy and Materials at the University of Birmingham.

The research group, currently comprising 6 graduate students with 3 post-doctoral fellows, uses first principles techniques to predict the structure and properties of materials for energy technologies.

The creation of new materials is both difficult and expensive. It is very difficult to "see" the structure of these materials over the length scales that they work and very expensive to create prototype materials to test. Whilst experimental physics can use X-rays, high-energy electrons or neutrons to infer the structure of these materials, this inference is made much more robust when combined with theoretical predictions of the kinds of structures that can be formed. In a computer we use quantum mechanical calculations to simulate the results of these kinds of experiments, helping to understand materials and suggest new materials with the kind of properties desired.

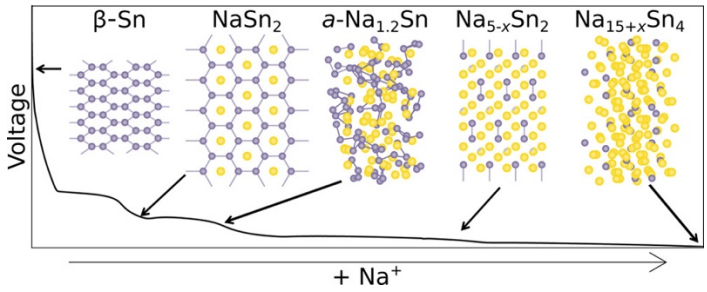
Our recent interest has been in electrodes for lithium-ion batteries [1]; novel charge carriers (beyond-Lithium) for batteries, such as sodium[2]; solid-state electrolytes[3]; and nano-phase change materials [4]. To do this, we use density-functional theory and global search techniques carrier out on the group's supercomputer along with university, regional and national supercomputers. We work closely with world-leading experimental groups to verify our predictions and aid further experiments. More details about the group may be found at: www.andrewjmorris.org

The project is anticipated to be a mix of code development, high-throughput computation and liaison with experimental collaborators. The precise project can be tailored somewhat to taste.

The candidate will have a 1st class Undergraduate or Masters degree (or equivalent) in Physics, Chemistry, Materials Science or related discipline. A strong background with programming (e.g. python, Fortran0X, C, C++), solid-state materials or electrochemistry would be advantageous.

Applications must be made through the university's on-line application system[5]: please provide a cover letter summarising your research interests and suitability for the position; the contact details of two people able to provide a letter of reference; and a full *curriculum vitae*. Please also send a copy of your full application to Andrew Morris directly.

Queries may be directed to Andrew Morris: a.j.morris.1@bham.ac.uk.



Schematic of the experimental discharge profile of a sodium-tin anode, showing how the voltage across the battery changes as sodium is added to it. Computation allows us to predict the phases of sodium-tin that form as sodium is included.
The $Na_{15}Sn_4$ phase carries over twice the charge of the standard lithium-ion battery anode. Sodium is about 100th of the cost to mine and refine than lithium.
[Figure reproduced under the CC-BY licence from reference [2]]

[1] Ab Initio Study of Phosphorus Anodes for Lithium- and Sodium-Ion Batteries, M. Mayo, K. J. Griffith, C. J. Pickard and A. J. Morris, Chem. Mater. ***28*** *2011-2021 (2016),*

[2] Investigating Sodium Storage Mechanisms in Tin Anodes: A Combined Pair Distribution Function Analysis, Density Functional Theory, and Solid-State NMR Approach, Joshua M. Stratford , Martin Mayo , Phoebe K. Allan, Oliver Pecher, Olaf J. Borkiewicz, Kamila M. Wiaderek, Karena W. Chapman,ä•, Chris J. Pickard, Andrew J. Morris, and Clare P. Grey, J. Am. Chem. Soc. ***139*** *7273-7286 (2017).*

[3] B. Karasulu and A. J. Morris, Unpublished (2017).

[4] Single-Atom Scale Structural Selectivity in Te Nanowires Encapsulated inside Ultra-Narrow, Single-Walled Carbon Nanotubes, Paulo V. C. Medeiros, Samuel Marks, Jamie M. Wynn, Andrij Vasylenko, Quentin M. Ramasse, David Quigley, Jeremy Sloan, and Andrew J. Morris, ACS Nano ***11*** *6178-6185 (2017).*

[5] http://bit.ly/2PGGcU9