UNIVERSITY OF BIRMINGHAM

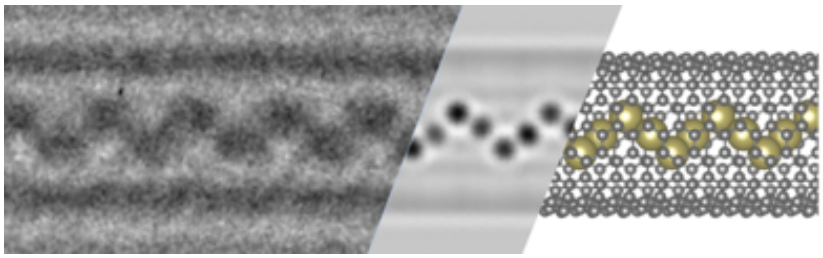
School of Metallurgy and Materials

PhD studentship in the Modelling of Nanoporous Materials: Digital Alchemy.

By tuning the size and properties of porous materials new chemical and physical reactions can be realised giving us unprecedented ability to tune catalysis, carbon capture, and energy storage reactions.

A 3-year competitively funded 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 using only computer simulation.



A 1D chain of tellurium inside a pore made from a carbon nanotube showing match between; (RHS) the ab initio prediction, (Middle) predicted TEM image and (LHS) experimental aberration corrected high-resolution transmission electron microscopy.

The crystal structures of new materials can be discovered using *ab initio* structure prediction techniques, such as AIRSS. Over the past several years the group has developed methods for the structure prediction of nanoporous materials including carbon nanotubes[1], metal-organic frameworks (MOFs)[2] and Zeolitic imidazolate framework (ZIFs). First principles spectroscopies such as EELS and NMR will be used to compare our predictions with experiment. 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. There will be many opportunities for international travel. 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 would be advantageous.

Applications must be made through the university's on-line application system[3]: 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.

[1] "Single-Atom Scale Structural Selectivity in Te Nanowires Encapsulated Inside Ultranarrow, Single-Walled Carbon Nanotubes", P. V. C. Medeiros, S. Marks, J. M. Wynn, A. Vasylenko, Q. M. Ramasse, D. Quigley, J. Sloan and A. J. Morris, *ACS Nano*, **2017**, *11* (6), pp 6178–6185, 10.1021/acsnano.7b02225

[2] "Experimental and Theoretical Evaluation of the Stability of True MOF Polymorphs Explains Their Mechanochemical Interconversions", Z. Akimbekov, A. D. Katsenis, G. P. Nagabhushana, G. Ayoub, M. Arhangelskis, A. J. Morris, T. Friščić, and A. Navrotsky, *J. Am. Chem. Soc.*, **2017**, *139* (23), pp 7952–7957, 10.1021/jacs.7b03144

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