A fully-funded 3.5 year PhD studentship is now available in the Karasulu Lab at Warwick.

**Project description:**
Nearing the theoretical limits of conventional Li-ion batteries, the ever-increasing demand for powering today’s energy-intensive applications has urged next-generation energy storage technologies. All-solid-state batteries (ASSBs), which utilise a solid electrolyte, have drawn soaring attention as they can (a) mitigate the safety risks associated with the conventional liquid electrolytes; and (b) provide superior battery performances. ASSBs will thus find uses in industries where battery safety and performance are utmost, such as electric vehicles. Some major limitations, however, are yet to be resolved before ASSBs can be fully commercialised, which we strive to tackle at a molecular level in our group through three closely-aligned work programmes run in parallel: (1) Discovering novel ASSB materials with superior performance; (2) Modelling the Solid-Solid Interfaces within ASSBs; and (3) Developing Atomic Layer Deposition (ALD) strategies for ASSB Applications.

The student will employ a wide range of state-of-the-art computational modelling methods, also contributing to their development. The research activities will involve the atomistic modelling and discovery of ASSB materials, and first-principles characterization of their various properties, which allow for a direct connection with the experiments, done by collaborators. These tasks require calculations that are run on local, and national-scale high-performance computing (HPC) facilities.

The work packages are implemented in close collaboration with the leading experimentalist and theoretician experts from the University of Warwick (Chemistry and WMG), University of Cambridge (Prof. Clare P. Grey and Prof. David J. Wales) and from abroad (TNO, Netherlands). The student will have ample chances (and expected) to interact with the collaborators during their appointment.

**Requirements:**
Applicants should have an honours degree (at least UK 2.1 or equivalent) in chemistry, physics, or material sciences. Prior experience in electronic structure theory, condensed matter theory, data analysis using Bash/Python/C++ scripts, software development (e.g. Python/, C++ or similar) and familiarity with Linux and high-performance computing (HPC) environments is highly advantageous, but not essential. The successful candidates will be initially trained on molecular modelling, data sampling and analytics methods. We certainly look for enthusiastic teammates who are eager to learn, create, and innovate in an ‘electrifying’ research field!

**Funding availability:** EU/UK (funded), non-UK (self-funded); only full-time employment

The studentship is funded through an EPSRC-Doctoral Training Programme (DTP) grant and it provides funding for 3.5 years that covers the maintenance and Home tuition fees, as well as a budget for the travel and training expenses along with a research support. The tax-free stipend is at the standard research council rates (currently £15,285 per annum, with annual increments). The student will not have any mandatory course load, however they will have access to the rich PhD-level training programme offered by the EPSRC/CDT-HetSys programme (more info can be found at https://warwick.ac.uk/fac/sci/hetsys/training/hetsystraining/). Non-UK applicants are welcome to apply, however they will need to arrange for additional funding for the full Band 2 Postgraduate Research fees (https://warwick.ac.uk/services/academicoffice/finance/fees/pgr/). Some funding opportunities are available for non-UK students (see https://warwick.ac.uk/about/brexit/future/), please contact us for further enquiries.

**How to apply:**
Please direct informal enquiries and requests for further information to Dr. Bora Karasulu (bora.karasulu @ warwick.ac.uk) Please include your CV (including contact details for at least two academic referees, and publications, if any) and a supporting statement (max 2 pages) detailing your interest in a PhD in the research area of the studentship and your suitability. Referees will be contacted at the interview stage, which is expected to take place in the week commencing July 4th.

Research group information is available at https://warwick.ac.uk/fac/sci/chemistry/staff/borakarasulu. Details on the formal application procedure can be found at http://www.go.warwick.ac.uk/pgapply.