

## 104065 - Research Fellow in Computational Chemistry/Energy Research - Chemistry

**Department: CHEMISTRY**

**Salary £30,942 – £36,914**

**Start Date: 1st September 2021 (or soon thereafter)**

**Full-time, Fixed-term for 36 months**

Apply Now

**A full-time 3-year PDRA position 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 packages 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.

We are looking for an enthusiastic post-doctoral researcher (PDRA) who is eager to learn, create, and innovate in an 'electrifying' research field! The postholder will have a background in computational chemistry, physics, computer science or other relevant discipline. They will employ a wide range of *state-of-the-art* computational modelling methods, also contributing to their development. The research activities 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 post is funded by an Engineering and Physical Sciences Research Council (EPSRC) grant.

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 PDRA will have ample chances (and is expected) to interact with the collaborators during their appointment.

**Selected Publications:** [1] *Physical Review Materials*, 2020, 4 (6), 065401; [2] *J. Am. Chem. Soc.*, 2020, 142, 6, pp. 3132-3148; [3] *Chem. Mater.* 2019, 31, 4, 1250-1257; [4] *ACS Nano*, 2017, 11 (9), 9303–9311; \*Copies are available upon request; also see this [profile](#).

Interviews are expected to take place week commencing the 18<sup>th</sup> July 2021.

If you have not yet been awarded your PhD but are near submission or have recently submitted your PhD, any offers of employment will be made as Research Assistant on level 5 of the University grade structure (£30,046). Upon successful award of your PhD and evidence of this fact, you will be promoted to Research Fellow on the first point of the level 6 of the University grade structure (£30,942).

### What we offer

We will provide you with a great range of benefits, which include an attractive pension scheme, 30 days' holiday plus Christmas closure, excellent learning and development opportunities, and savings on a wide range of products and services. We offer a generous maternity/paternity/adoption/parental leave policy, onsite childcare facilities. We recognise the importance of a healthy work/life balance and offer you access to flexible working, for more information visit our [Rewards and Benefits webpage](#).

We also have an excellent relocation package; to assess whether you may be entitled, please see details on the following page <https://warwick.ac.uk/services/humanresources/vacancies/relocation/>.


### Athena SWAN Silver Award

We are committed to supporting staff to achieve their potential. Both the Department of Chemistry and the University of Warwick hold Athena SWAN silver awards, a national initiative that recognises the advancement of gender equality, representation, progression, and success for all in academia. We provide a welcoming and inclusive working and learning environment, recognising that everyone is different in a variety of visible and non-visible ways, and that those differences are to be recognised, respected, and valued. We welcome applications from individuals who identify with any of the protected characteristics defined by the Equality Act 2010. We are supportive of staff with caring responsibilities.

## Job Description

### Job Purpose (A brief summary of the role):

The post-doctoral researcher (PDRA) will employ a wide range of *state-of-the-art* computational modelling methods to model all-solid-state battery (ASSB) materials, viz. electrodes and electrolytes, and related coating materials. The PDRA will use both DFT and empirical potential based methods to (a) investigate various structural, electronic, and spectroscopic properties of the battery materials; (b) explore new materials through high-throughput computational screening; (c)



model the solid-solid interfaces and their chemistry and (d) predict the ionic and electronic transport behaviour within bulk materials and at the interfaces. Ideally, the post holder will also contribute to the development of the computational methodology, working on the group codes and writing input preparation and post-analysis scripts. The PDRA will therefore need to run calculations on local, and national-scale high-performance computing (HPC) facilities.

### **Duties and Responsibilities:**

1. Apply computational techniques (based on both DFT and empirical potentials) for (a) the modelling of battery materials and their various properties as well as their interfaces; (b) exploration of new materials and (c) the prediction of ionic and electronic transport behaviour within bulk materials and their interfaces.
2. Contribute to the preparation of peer-reviewed publications, posters, and scientific reports,
3. Deliver oral and poster presentations at national/international conferences and workshops.
4. Participate in group seminars, collaboration meetings, and other intellectual activities.
5. Assist in the supervision of MSc and PhD students affiliated to the project
6. Manage own academic research and administrative activities, including small-scale project management and coordinating multiple aspects of work to meet deadlines.
7. To act with professionalism at all times and show respect to their colleagues and to understand and adhere to the University's value of dignity at work; they are also expected to work collegially and to support all the teams with which they have contact in achieving the University's objectives.
8. Any other duties commensurate with the grade and level of responsibility of this post, for which the post holder has the necessary experience and/or training.

## Person Specification

The Person Specification focuses on the knowledge, skills, experience and qualifications required to undertake the role effectively. This is measured by (a) Application Form, (b) Publication Sample, (c) Interview, (d) Presentation.

### Essential Criteria

- 1.\* Applicants must have (or expect to shortly obtain) a PhD in a relevant area of computational chemistry, physics, computer science or other relevant discipline; (a)

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Competence in computational chemistry applications using density-functional
- 2.\* theory and empirical interatomic potentials, large data analysis using shell/Python scripts, and/or scientific programming (e.g. Python/, C++ or similar) (a), (b), (c), (d)

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3. A demonstrated capacity for independent research work. (a), (b), (c), (d)

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4. The candidate should have an emerging track record of peer-reviewed publications of disseminating results at conferences, as demonstrated by co-/first author contributions. (a), (b)

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5. Effective written and verbal communication skills in English. (a), (b), (c), (d)

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6. An ability to work collaboratively and effectively with academic and administrative colleagues, and with colleagues outside the University to promote collegiality. (a), (c)

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## Desirable Criteria

1. Proven experience in the application of first-principles methods, theoretical spectroscopy, and/or molecular dynamics as well as developing scientific codes is highly desirable. (a), (b), (c)

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2. A strong background in electronic structure theory, condensed matter theory, electrochemistry and/or surface chemistry will be advantageous. (a), (c)

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3. Experience in using high performance computing (HPC) in a Unix/Linux environment, command line tools and shell scripting is highly desirable. (a), (c)

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4. Familiarity with application/development of machine-learning based interatomic potentials will be advantageous. (a), (c)

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5. Ability and willingness to write bids for grant and compute (HPC) time proposals is desirable (a), (c)

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## Further Particulars

Please include your CV, contact details for at least three academic referees, your publication and presentations list, one key publication (if any) and a supporting statement (max 2 pages) detailing your interest in the research area and your suitability for the role. This information should be submitted with your online application.

Referees may be contacted at the interview stage prior to consent.

Please direct informal enquiries and requests for further information to Dr. Bora Karasulu (bora.karasulu {at} warwick.ac.uk).

Research group information is available at

<https://warwick.ac.uk/fac/sci/chemistry/staff/borakarasulu>.

For further information about the University of Warwick, please read our [University Further Particulars](#).

For more information about the department please see [www.warwick.ac.uk/go/chemistry](http://www.warwick.ac.uk/go/chemistry)

A summary of the facilities available to Warwick Chemistry are given in

<http://www2.warwick.ac.uk/fac/sci/chemistry/research/chemistryoverview>

<http://www2.warwick.ac.uk/fac/sci/chemistry/research/>