

| Job title | b title Research Associate/Fellow | | Research and Teaching Level 4 (Appointment will be Level 4 Career training grade where an appointment is made before PhD has been completed) | |
|-----------------------|--|----------|---|--|
| School/ Department | Faculty of Engineering – Advanced Materials Research Group | Location | Research Acceleration and Demonstration (RAD) Building, Jubilee Campus | |

Purpose of role

We are recruiting a Research Associate/Fellow for the Hydrogen Research Group currently consisting of 5 academics, 9 research fellows and 15 PhD students. The successful applicant will be joining a multidisciplinary research team collaborating on the optimisation of metal hydrides and/or the design of solid-state hydrogen stores and compressors.

The role will focus on code development for the modelling of metal (complex) hydrides using machine learning techniques.

| | Main responsibilities (Primary accountabilities and responsibilities expected to fulfil the role) | % time per year |
|---|---|-----------------------|
| 1 | To plan and conduct research using recognised computational approaches, methodologies and techniques within the research area. | 50% |
| 2 | To analyse and illuminate data, interpret reports, evaluate and criticise texts and bring new insights to research area. | 15% |
| 3 | To write up research work for publication and/or contribute to the dissemination at national/international conferences, resulting in successful research outputs. | 15% |
| 4 | To provide introductions, support, guidance and supervision to other staff. | 10% |
| 5 | To provide supervision of UG/PGT project students and PhD students; training/mentoring for junior researchers; STEM outreach; being engaged with an interest group (examples Engineering Research Futures, researcher groups, BME Staff Network, Ignite EDI Network+) | 5% |
| 6 | Miscellaneous: You may occasionally be asked to perform other duties which are not included in the above but appropriate to the grade and consistent with the role | 5% |

Person specification

| | Essential | Desirable |
|---|---|--|
| Skills | Proven research skills, especially in computational materials science Ability to analyse and write up data Excellent communication and presentation skills Excellence at writing in the English language Well organised and self-motivated, able to work independently and as part of a team | |
| Knowledge and experience | Advanced knowledge in atomistic computational modelling of solid-state materials using machine learning interatomic potentials Experience in developing or adapting Python codes to train machine learning interatomic potentials of solid-state materials Experience in running molecular dynamics simulations using machine learning interatomic potentials and analysing the simulation results Experience with the interpretation of relevant experimental data Contributed to new understanding in the field of hydrogen or energy research. | Experience in using ab initio density functional theory packages such as VASP, CP2K, etc |
| Qualifications, certification and training (relevant to role) | PhD or about to obtain (or equivalent) in an appropriate field (e.g. Chemistry, Physics or Materials Science, or a related discipline) | |











Expectations and behaviours

The University has developed a clear set of core expectations and behaviours that our people should be demonstrating in their work, and as ambassadors of the University's strategy, vision and values. The following are essential to the role:

Valuing people Is friendly, engaging and receptive, putting others at ease.

Actively listens to others and goes out of way to ensure people

feel valued, developed and supported.

Taking ownership Is clear on what needs to be done encouraging others to take

ownership. Takes action when required, being mindful of important aspects such as Health & Safety, Equality, Diversity &

Inclusion, and other considerations.

Forward thinking Drives the development, sharing and implementation of new

ideas and improvements to support strategic objectives. Engages

others in the improvement process.

Professional pride Is professional in approach and style, setting an example to

others; strives to demonstrate excellence through development of

self, others and effective working practices.

Always inclusive Builds effective working relationships, recognising and including

the contribution of others; promotes inclusion and inclusive

practices within own work area.

Key relationships with others

