



Job title	Research Associate/Fellow	Job family and level	Research and Teaching Level 4
School/ Department	Faculty of Engineering – Advanced Materials Research Group	Location	Research Acceleration and Demonstration (RAD) Building, Jubilee Campus

Purpose of role

We are seeking a highly motivated Research Associate/Fellow to join the Hydrogen Research Group at the University of Nottingham. The successful candidate will become part of a multidisciplinary team of scientists and engineers working at the forefront of hydrogen materials research. The project will focus on the optimisation of metal (complex) hydrides and the development of advanced solid-state hydrogen storage and compression technologies. A key aspect of the role will be the computational discovery, design, and modelling of metal (complex) hydrides using state-of-the-art atomistic and data-driven approaches.

	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 and experience in atomistic computational modelling of solid-state materials using density functional theory and/or machine learning interatomic potentials • Experience with at least one of the following techniques: (1) developing or adapting Python codes to train machine learning interatomic potentials of solid-state materials; (2) computational high throughput screening of materials (e.g. using machine learning methods); (3) Calphad; (4) phase-field modelling. • Experience with interpretation of relevant experimental data	• Experience in using ab initio density functional theory packages such as VASP, CP2K, etc • Experience in running molecular dynamics simulations using machine learning interatomic potentials and analysing the simulation results • Experience in using AI agent for materials modelling and discovery
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

