



Job title	Research Associate/ Fellow in Modelling of next generation hydrogen storage materials	Job family and level	Research and Teaching Level 4a +
School/ Department	Faculty of Engineering - Advanced Materials Research Group	Location	Jubilee Campus

Purpose of role

Based in the Advanced Materials Research Group within the Faculty of Engineering, the successful candidate will work with Dr Sanliang Ling and Prof Martin Dornheim to perform computational modelling on metal hydrides and metal complex hydrides for energy storage applications. The successful candidate will computationally study metal hydrides and complex hydride based materials in order to understand the structure-property relationship. They will also use the fundamental understanding to design new metal (complex) hydride materials for selected energy storage applications.

	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.	25%
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.	15%
5	Contribution to organization of research resources and facilities, as well as seminars	10%
6	To build and maintain relationships with both internal and external contacts in order to exchange information, to form relationships for future collaborations and identify potential sources of funds and/or opportunities for collaboration.	5 %
7	To co-ordinate the operational aspect of research networks, for example, arranging meetings and updating web sites etc and contribute to collaborative decision making with colleagues in area of research.	5 %
8	To develop research objectives and proposals for own and/or collaborative research area.	5 %
9	Any other duties appropriate to the role as required by the line manager.	5%

Person specification

	Essential	Desirable
Skills	<ul style="list-style-type: none"> • 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	<ul style="list-style-type: none"> • Advanced knowledge of computational solid-state chemistry or materials science methods • Proven research record in atomistic computational modelling of solid-state materials, Calphad or phase-field modelling • Strong publication track record • Experience with the interpretation of relevant experimental data • Demonstrated creativity and leadership in problem solving 	<ul style="list-style-type: none"> • Research experience on metal hydrides or metal complex hydrides • Experience in using a variety of ab initio density functional theory packages, such as VASP, CP2K, etc • Experience with computational high throughput screening of materials (e.g. using machine learning methods) • Experience with Calphad and/or phase-field modelling • Experience with scripting languages (e.g. Python) and workflow packages (e.g. ASE and Pymatgen) • Experience of multi-disciplinary working and communication with experimental scientists
Qualifications, certification and training (relevant to role)	<ul style="list-style-type: none"> • PhD or near completion (or equivalent) in an appropriate field (e.g. Chemistry, Physics or Materials Science, or a related discipline) 	



The University strongly endorses Athena SWAN principles, with commitment from all levels of the organisation in furthering women's careers. It is our mission to ensure equal opportunity, best working practices and fair policies for all.

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 always equitable and fair and works with integrity. Proactively looks for ways to develop the team and is comfortable providing clarity by explaining the rationale behind decisions.
- Taking ownership** Is highly self-aware, looking for ways to improve, both taking on board and offering constructive feedback. Inspires others to take accountability for their own areas.
- Forward thinking** Driven to question the status quo and explore new ideas, supporting the team to "lead the way" in terms of know-how and learning.
- Professional pride** Sets the bar high with quality systems and control measures in place. Demands high standards of others identifying and addressing any gaps to enhance the overall performance.
- Always inclusive** Ensures accessibility to the wider community, actively encouraging inclusion and seeking to involve others. Ensures others always consider the wider context when sharing information making full use of networks and connections.

Key relationships with others

