



Job Description

Job title:	Postdoctoral Researcher in Atomistic and DFT Modelling of Lithium Batteries
Department/School:	Chemistry
Grade:	7
Location:	Department of Chemistry, 1South

Job purpose

The research programme will apply atomistic and ab initio techniques in the study of defect, transport and surface/interface properties of lithium battery materials. Project areas will include ion intercalation at electrode surfaces and effects of grain boundaries using potentials-based molecular dynamics, cluster expansion based Monte Carlo and DFT techniques. These projects form part of the large interdisciplinary Multi-Scale Modelling effort on lithium batteries within the new Faraday Institution with strong links to continuum modelling work, and to experimental structural and electrochemical studies.

Source and nature of management provided

Prof Saiful Islam & Dr Benjamin Morgan

Staff management responsibility

None, although day to day assistance/supervision of other group members e.g. PhD and/or undergraduate students may be required.

Career and Professional Development Activities

From time to time you may be asked to assist in the facilitation of CPD activities.

Special conditions

Compliance with all relevant Codes of Practice and regulations for the University and relevant discipline.

Main duties and responsibilities

- | | |
|----------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 1 | To apply computational techniques (DFT, potentials-based MD, and effective-potential MC methods) for the modelling of battery materials. |
| 2 | To apply computational techniques in the study of defect, transport, and electronic properties within the bulk and at surfaces. To link up with continuum modelling work as part of a large multi-scale modelling effort on lithium batteries. |
| 3 | To prepare papers for publication in high quality international journals. |
| 4 | To appropriately manage research data and analysis software for archival and publication. |
| 5 | To give presentations at conferences. |
| 6 | To participate in meetings with research collaborators. |
| 7 | To assist in the supervision of PhD students within the research groups. |
| 8 | To undertake other duties required by the research team |

You will from time to time be required to undertake other duties of a similar nature as reasonably required by your line manager.



Person Specification

Criteria	Essential	Desirable	Assessed by		
			A/F	I	R
Qualifications					
PhD in Chemistry, Physics, Materials Science or a related discipline	Y		X		
Experience/Knowledge					
Solid state chemistry or materials science	Y		X	X	
Computer modelling of solid state materials (expertise ideally includes some or all of DFT, potentials-based MD, cluster-expansion-based MC)	Y		X	X	
Knowledge of solid state materials research in the area of energy materials, with specific focus on battery materials.	Y		X	X	X
Previous postdoctoral research experience		Y	X	X	X
Good track record of writing and publishing peer-reviewed papers – especially as main author	Y			X	X
Track record of conference talks.	Y		X		
Experience developing software as part of a team.		Y	X	X	X
Skills					
Computer modelling techniques as applied to solid-state battery materials (DFT and/or potentials-based)	Y		X	X	
Good communication skills e.g. written skills in the application form, talks and writing papers as main author	Y		X	X	
Good interpersonal skills	Y			X	
Good general scientific computing skills, e.g. scripting / programming in appropriate languages (Fortran, Python, or equivalent).		Y	X	X	

Appendix B

Attributes					
Have the ability to work independently	Y		X	X	X
Team worker		Y		X	X
Flexibility in changes in the research programme	Y			X	X

Code: A/F – Application form, I – Interview, R – Reference