Job Description

Job title:	**Many-body electrical and optical modelling of solar cells**
Department/School:	**Department of Chemistry**
Grade:	**EU FP7 Early Career Researcher**
Location:	**Department of Chemistry, University of Bath**

Job purpose
To conduct research in computational materials science as part of an EU funded Initial Training Network, DESTINY.

Source and nature of management provided
Dr. Aron Walsh, Royal Society University Research Fellow, is the PI of the project and will give guidance over research activities.

Staff management responsibility
None.

Career and Professional Development Activities
The post holder will be able to attend courses organised by the Graduate School and Staff Development in various areas of teaching, research and generic skills related activities. *From time to time you may be asked to assist in the facilitation of CPD activities. This will form part of your substantive role and you will not receive additional payment for these activities.*

Special conditions
N/A

Main duties and responsibilities
High-quality research will be conducted as part of a project on the development of more stable and efficient dye-sensitised solar cells. *This position will focus on developing simulations of the surface structure of TiO_2, adsorption of novel dye molecules and the interface with the redox electrolyte. This will involve the application of large-scale density functional theory*

techniques, and an emphasis will be placed on the calculation of optical, vibrational and electronic spectroscopic data to interpret experimental measurements from our partner groups.	
1	To contribute to the programme of research, including large-scale electronic structure calculations on the UK's supercomputer HECToR (> 90,000 cores).
2	To contribute to the programme of collaborative research with the DESTINY network.
3	To record, analyse and write up the results.
4	To contribute to the drafting and submitting of papers to peer-reviewed journals.
5	To prepare progress reports on research for funding bodies as required.
6	To contribute to the preparation and drafting of research bids and proposals.
7	To undertake a limited amount of teaching in relation to the subject area.
8	Dissemination of research results at national and international conferences.
9	To contribute to the induction and direction of other research staff and students as requested.
10	Responsible for ensuring that equipment is safe and maintained in working order.
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/T	R
Qualifications					
First-class Masters degree in Chemistry or Physics.	X		X	X	
Experience/Knowledge					
Knowledge of a range of computational research techniques, including electronic structure (e.g. DFT, HF) methods applied to the treatment of molecular or solid-state systems.	X		X	X	
Knowledge of *ab initio* thermodynamics.	X		X	X	
Strong recent publication record.		X	X	X	
Practical experience in calculations the optical properties of solids or spectroscopic response.		X	X	X	
Skills					
Proven record of ability to conduct high quality research, as reflected by the authorship of publications or other research outputs, in areas including computational or theoretical materials science, solid-state or materials chemistry/physics.	X		X		X
Fluency in scientific English.	X		X	X	X
Working knowledge of the Fortran programming language or the equivalent.	X		X	X	
Practical experience of High Performance Computing platforms.		X	X	X	
Practical experience using the DFT codes VASP, CASTEP, FHI-AIMS or similar.	X		X	X	

Attributes					
Versatility, innovation and the ability to work in a multidisciplinary team	X		X	X	
Commitment to excellence in research	X		X	X	
Commitment to safe working practices	X		X	X	
Commitment to working within professional/ethical codes of conduct	X		X	X	

Code: A/F – Application form, I/T – Interview/Test, R – References