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| Last updated: | 12/02/2019 |

**JOB DESCRIPTION**

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| Post title: | **Research Fellow** |
| School/Department: | Chemistry |
| Faculty: | Faculty of Engineering and Physical Sciences (FEPS) |
| Career Pathway: | Education, Research and Enterprise (ERE) | Level: | 4 |
| \*ERE category: | Research pathway |
| Posts responsible to: | Prof of Computational Chemistry |
| Posts responsible for: | ---- |
| Post base: | **Office-based** |

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| Job purpose |
| To develop theory and code for multiscale and large scale quantum mechanical methods in the ONETEP code for linear-scaling electronic structure calculations and other codes. To contribute to exemplar simulations on battery materials and interfaces using the developed approaches. To undertake leadership, management and engagement activities. |

| Key accountabilities/primary responsibilities | % Time |
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|  | To develop and carry out an area of personal research.  | 50 % |
|  | Regularly disseminate findings by taking the lead in preparing publication materials for referred journals, presenting results at conferences, or exhibiting work at other appropriate events. | 10 % |
|  | Contribute to the writing of bids for research funding. | 5 % |
|  | Investigate models and approaches to test and develop them. | 5 % |
|  | Collaborate/work on original research tasks with colleagues in other institutions. | 15 % |
|  | Carry out administrative tasks associated with specified research funding, for example risk assessment of research activities, organisation of project meetings and documentation. Implementation of procedures required to ensure accurate and timely formal reporting and financial control. | 2 % |
|  | Supervise the work of junior research staff. | 5 % |
|  | Carry out occasional undergraduate supervision, demonstrating or lecturing duties within own area of expertise, under the direct guidance of a member of departmental academic staff. | 5 % |
|  | Any other duties as allocated by the line manager following consultation with the post holder. | 3 % |

| Internal and external relationships |
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| Internal relationships:* To provide guidance to staff and students.
* To undertake instruction of undergraduate project students or PhD students as agreed.

External relationships* The project is a collaboration with Merck. The appointee will need to collaborate closely with them.
* To participate in and help organise project meetings.
* To develop contacts and research collaborations within the University and the wider community.
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| Special Requirements |
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| To be available to participate in fieldwork as required by the specified research project. To attend national and international conferences for the purpose of disseminating research results.To undertake secondment periods at Merck.*Applications for Research Fellow positions will be considered from candidates who are working towards or nearing completion of a relevant PhD qualification. The title of Research Fellow will be applied upon successful completion of the PhD. Prior to the qualification being awarded the title of* ***Senior Research Assistant*** *will be given.* |

**PERSON SPECIFICATION**

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| Criteria | Essential | Desirable | How to be assessed |
| Qualifications, knowledge and experience | PhD or equivalent professional qualifications and experience in computational chemistry, materials or physics.Experience in using plane-wave pseudopotential codes and/or localised basis set (e.g Gaussian basis set) codes.Demonstrated programming experience in electronic structure theory. Ability to understand linear-scaling methods for first principles quantum mechanical calculations in detail.Publications in the development and application of DFT and experience of DFT calculations.  | Understanding of best practice in software development.Experience in doing simulations with DFT.Experience in doing simulations of materials with atomistic methods | CV/InterviewCV/InterviewCV/InterviewCV/Interview |
| Planning and organising | Ability to conduct a detailed review of recent literature.Ability to develop and apply new concepts.Creative approach to problem-solving.Ability to organise own work with minimal supervision.Ability to prioritise own work in response to deadlines. |  | CV/InterviewCV/InterviewCV/InterviewCV/InterviewCV/Interview |
| Problem solving and initiative | High level analytical capability.Ability to apply relevant models, techniques and methods and develop new ones.Ability to assess resource requirements and deploy them effectively. |  | InterviewInterviewInterview |
| Management and teamwork | Must possess strong inter-personal skills - ability to deal with a wide range of people.Ability to direct the work of a small research team and motivate others to produce a high standard of work. |  | InterviewCV/Interview |
| Communicating and influencing | Communicate new and complex information effectively, both verbally and in writing, engaging the interest and enthusiasm of the target audienceAble to present research results at group meetings and conferencesAble to write up research results for publication in leading peer-viewed journalsWork proactively with colleagues in other work areas/institutions, contributing specialist knowledge to achieve outcomes | Ability to encourage research culture in others. | CVCV/InterviewInterview |
| Other skills and behaviours | Positive attitude to colleagues and students | Advanced computer programming skills. | CVInterview |
| Special requirements | Ability to take the lead in the dissemination of results by submitting publications to refereed journals, participating in relevant electronic structure and battery materials simulation networks and attending conferences and project meetings. Play an active role in the Department and will be expected to interact with external collaborators.Required to be present in the office at least during the core working hours of the Skylaris group.  |  | CV/InterviewInterview |

**JOB HAZARD ANALYSIS**

**Is this an office-based post?**

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| [x]  Yes | If this post is an office-based job with routine office hazards (eg: use of VDU), no further information needs to be supplied. Do not complete the section below. |
| [ ]  No | If this post is not office-based or has some hazards other than routine office (eg: more than use of VDU) please complete the analysis below.Hiring managers are asked to complete this section as accurately as possible to ensure the safety of the post-holder. |

## - HR will send a full PEHQ to all applicants for this position. Please note, if full health clearance is required for a role, this will apply to all individuals, including existing members of staff.

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| **ENVIRONMENTAL EXPOSURES** | **Occasionally** (<30% of time) | **Frequently**(30-60% of time) | **Constantly**(> 60% of time) |
| Outside work  |  |  |  |
| Extremes of temperature (eg: fridge/ furnace) |  |  |  |
| ## Potential for exposure to body fluids |  |  |  |
| ## Noise (greater than 80 dba - 8 hrs twa) |  |  |  |
| ## Exposure to hazardous substances (eg: solvents, liquids, dust, fumes, biohazards). Specify below: |  |  |  |
| Frequent hand washing |  |  |  |
| Ionising radiation  |  |  |  |
| **EQUIPMENT/TOOLS/MACHINES USED** |
| ## Food handling  |  |  |  |
| ## Driving university vehicles(eg: car/van/LGV/PCV)  |  |  |  |
| ## Use of latex gloves (prohibited unless specific clinical necessity) |  |  |  |
| ## Vibrating tools (eg: strimmers, hammer drill, lawnmowers)  |  |  |  |
| **PHYSICAL ABILITIES** |
| Load manual handling |  |  |  |
| Repetitive crouching/kneeling/stooping |  |  |  |
| Repetitive pulling/pushing |  |  |  |
| Repetitive lifting |  |  |  |
| Standing for prolonged periods |  |  |  |
| Repetitive climbing (ie: steps, stools, ladders, stairs) |  |  |  |
| Fine motor grips (eg: pipetting) |  |  |  |
| Gross motor grips |  |  |  |
| Repetitive reaching below shoulder height |  |  |  |
| Repetitive reaching at shoulder height |  |  |  |
| Repetitive reaching above shoulder height |  |  |  |
| **PSYCHOSOCIAL ISSUES** |
| Face to face contact with public |  |  |  |
| Lone working |  |  |  |
| ## Shift work/night work/on call duties  |  |  |  |