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| Last updated: | May 2020 |

**JOB DESCRIPTION**

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| Post title: | **Senior Research Fellow** | | |
| School/Department: | Chemistry | | |
| Faculty: | Engineering and Physical Sciences | | |
| Career Pathway: | Education, Research and Enterprise (ERE) | Level: | 5 |
| \*ERE category: | Research pathway | | |
| Posts responsible to: | Principal Investigator | | |
| Posts responsible for: | n/a | | |
| Post base: | Office-based/Non Office-based (see job hazard analysis) | | |

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| Job purpose |
| To plan and deliver research in accordance with the specified research project under the supervision of the project director. To undertake leadership, management and engagement activities. |

| Key accountabilities/primary responsibilities | | % Time |
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|  | Plan and deliver high quality research within a specified area, assisting in project management of the research activity, sustaining a personal research plan, and supervising and taking responsibility for the research team. This will include computational research on molecular crystals, including evolutionary exploration and other generative models for promising identifying molecules. | 50% |
|  | Establish a national reputation by sustaining the regular dissemination of findings through leading peer-reviewed publications, presenting results at conferences, or exhibiting work at other appropriate events. |
|  | Plan and develop innovative research projects. |
|  | Develop and engage in research methodologies that add to the knowledge/understanding of the subject area. Lead the development, testing and documentation of computational chemistry software developed in the research group. | 45% |
|  | Collaborate on and develop original research with colleagues in other institutions, including planning, coordination and work on integration of computation and lab automation with colleagues in other institutions. |
|  | Carry out management and administrative tasks associated with specified research funding, including risk assessment of project activities, organisation of project meetings and documentation and preparation of annual reports. To oversee and implement procedures required to ensure accurate and timely formal reporting and the safe archiving of research data. |
|  | Undertake liaison with external organisations including equipment manufacturers, steering committees, associated academic facilities and commercial users. |
|  | Provide expert advice in own subject area to other staff and students. |
|  | Carry out occasional student supervision within own area of expertise. |
|  | Any other duties as allocated by the line manager following consultation with the post holder. | 5% |

| Internal and external relationships |
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| Responsibility to research award holder/project director.  Responsibility for reporting and liaison to external funding bodies or sponsors.  As a senior member of the project team, will coordinate the day-to-day activities of research and technician staff under the guidance of the project director.  Collaborators and colleagues in other work areas and institutions. |

| 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. |

**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 Chemistry, Materials Science, Physics or a related area.  Significant postdoctoral research experience in computational chemistry or a related field.  Track record of published research  Excellent computing skills.  Programming experience  Experience with management of software development. | Use of high-performance computing facilities.  Experience in automating large scale calculations.  Experience with materials modelling.  Experience with force field-based simulations.  Experience with solid state quantum mechanical simulations.  Experience with use of, or development of, machine learning methods.  Experience in programming in Python.  Experience with database management.  Research experience in an interdisciplinary project.  Experience of applying computational methods to materials  Experience of managing software development and experience in contributing to large software projects. | Application form, references, and interview |
| Planning and organising | Proven ability to organise a range of high quality research activities to deadline and quality standards, ensuring plans complement broader research strategy  Proven ability to develop innovative research proposals and attract research funding | Able to build a research team | Application form, references, and interview |
| Problem solving and initiative | Able to identify broad trends to assess deep-rooted and complex issues  Able to apply originality in modifying existing approaches to solve problems |  | Interview |
| Management and teamwork | Able to manage, motivate and coordinate research team, delegating effectively. Able to formulate staff development plans, if appropriate  Able to undertake coordinating role in School/Department/university  Able to monitor and manage resources and budgets  Work effectively in a team, understanding the strengths and weaknesses of others to help teamwork development |  | Application form, references, and interview |
| Communicating and influencing | Communicate new and complex information effectively, both verbally and in writing, engaging the interest and enthusiasm of the target audience  Track record of presenting research results at group meetings and conferences  Able to persuade and influence at all levels in order to foster and maintain relationships  Able to resolve tensions/difficulties as they arise  Able to provide expert guidance to colleagues in own team, other work areas and institutions to develop understanding and resolve complex problems |  | Application form, references, and interview |
| Other skills and behaviours | Compliance relevant Health & Safety issues  Proactive in promoting a working environment that is inclusive and engaging; recognising the value diversity brings. |  | Interview |
| Special requirements | Able to attend national and international conferences to present research results |  | Application, interview |

**JOB HAZARD ANALYSIS**

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

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| 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 |  |  |  |