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| Last updated: | 11/8/2023 |

**JOB DESCRIPTION**

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| Post title: | **Research Fellow in Computational Materials Discovery** | | |
| School/Department: | School of Chemistry | | |
| Faculty: | Faculty of Engineering and Physical Sciences | | |
| Career Pathway: | Education, Research and Enterprise (ERE) | Level: | 4 |
| \*ERE category: | Research pathway | | |
| Posts responsible to: | Graeme Day (Level 7) | | |
| Posts responsible for: | N/A | | |
| Post base: | Office-based | | |

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| Job purpose |
| This post is part of an ambitious 6-year project, ADAM – Autonomous Discovery of Advanced Materials. The ADAM project is a collaboration between the computational materials chemistry group, led by Prof. Graeme Day at the University of Southampton, and groups at the Universities of Liverpool (Professor Andrew Cooper) and Rostock (Professor Kerstin Thurow). The goal is the development of methods for accelerating the discovery of materials through the development of predictive computational methods and their use to inform automated experiments.  The researcher on this post will work with crystal structure prediction and chemical space exploration methods for identifying crystalline molecular materials with promising properties, and will develop methods for analysing large data sets from these simulations to develop structure-function relationships. The researcher will collaborate with chemists in collaborating institutions to integrate computational methods with experimental studies.  The researcher’s responsibilities include method development and testing, design and running of large-scale calculations and documentation of code. The post holder will analyse and interpret data, prepare written and oral reports on progress and contribute to the preparation of applications for high performance computing time. The researcher will contribute to the whole vision of the project, including the direction for developments in computation, robotics and materials characterisation, through regular team meetings. |

| Key accountabilities/primary responsibilities | | % Time |
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|  | To carry out computational research on molecular crystals, including crystal structure prediction, evolutionary algorithms for exploring chemical space, machine learning to analyse the resulting structure-property space. | 65 % |
|  | To contribute to the testing and documentation of computational chemistry software developed in the research group. | 8 % |
|  | Regularly disseminate findings by taking the lead in preparing publication materials for refereed journals, presenting results at conferences, or exhibiting work at other appropriate events. | 5 % |
|  | Ensuring the effective and safe archiving of research data. | 2 % |
|  | Assistance and training of postgraduate students and junior group members. | 5 % |
|  | Collaborate/work on original research tasks with colleagues in other institutions. | 10 % |
|  | Carry out occasional undergraduate supervision or demonstrating, under the direct guidance of a member of departmental academic staff. | 2 % |
|  | Any other duties as allocated by the line manager following consultation with the post holder. | 3 % |

| Internal and external relationships |
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| Direct responsibility to holder of research award.  The researcher will report directly to Prof. Graeme Day (GD) and will verbally report on research progress to all members of the research team, including collaborators at the Universities of Liverpool and Rostock. The researcher will provide regular, clear verbal and written progress reports to the research group leader (GD). Will interact effectively with the wider research team. |

| Special Requirements |
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| To be available to attend national and international conferences for the purpose of disseminating research results. To participate in meetings in the UK and Europe with collaborators.  To assist the PI in the management of the laboratory.  *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 Chemistry, Materials Science, Physics or a related area.  Good computing skills.  Detailed understanding and knowledge of computational chemistry methods. | Use of high performance computing facilities.  Experience in running and automating large scale calculations.  Experience with materials modelling.  Experience with use of, or development of, methods for analysing large-scale computational data, including machine learning methods.  Programming experience.  Experience with Python | Application form, references, and interview |
| Planning and organising | Able to organise own research activities to deadline and quality standards. |  | interview |
| Problem solving and initiative | Able to develop understanding of complex problems and apply in-depth knowledge to address them  Willingness to learn new skills and ability to develop original techniques/methods |  | interview |
| Management and teamwork | Able to supervise work of junior research staff, including postgraduate students, delegating effectively.  Work effectively in a team, understanding the strengths and weaknesses of others to help teamwork development. | Previous interdisciplinary work. | 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.  Able to present research results at group meetings and conferences.  Able to write up research results for publication in leading peer-viewed journals.  Work proactively with colleagues in other institutions, contributing specialist knowledge to achieve project outcomes. | Strong publication record. | Application form, references, and interview |
| Other skills and behaviours | Understanding of relevant Health & Safety issues.  Positive attitude to colleagues and students. |  | interview |
| Special requirements | Able to attend national and international conferences to present research results.  Able to travel for short visits to research collaborators within the UK and Europe. |  | 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 |  |  |  |