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| Last updated: | 19/5/2020 |

**JOB DESCRIPTION**

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| Post title: | **Research Fellow in Digital 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: | Professor of Chemical Modelling | | |
| Posts responsible for: | N/A | | |
| Post base: | Office-based | | |

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| Job purpose |
| This post is part of the EPSRC-funded “Programme Grant Digital navigation of chemical space for function”, a collaboration between research groups at the Universities of Southampton, Liverpool and Imperial College London. This project aims to transform our ability to access functional materials with unprecedented chemical and structural diversity by fusing physical and computer science, by developing a digital discovery.  The goal of this position is to develop the use of crystal structure prediction methods for organic molecules to accelerate the discovery of materials, informing experimental discovery programmes which includes automation in the lab. The researcher’s responsibilities include the design and running of large-scale calculations, incorporating machine learning into simulations and analysis, software development and documentation, as well as coordination between collaborating research groups. 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 |
| --- | --- | --- |
|  | To lead the development, testing and documentation of computational chemistry software developed in the research group. | 40 % |
|  | Plan, coordinate and work on integration of computation and lab automation with colleagues in other institutions. |
|  | Carry out occasional undergraduate supervision or demonstrating, under the direct guidance of a member of departmental academic staff. |
|  | To carry out computational research on molecular crystals, including large-scale crystal structure prediction, evolutionary exploration and other generative models for promising identifying molecules. | 40 % |
|  | 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. | 15 % |
|  | Ensuring the effective and safe archiving of research data. |
|  | Assistance and training of postgraduate students and junior group members. |
|  | Any other duties as allocated by the line manager following consultation with the post holder. | 5 % |

| Internal and external relationships |
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| Direct responsibility to holder of research award.  The researcher will report directly to the Professor of Chemical Modelling and will verbally report on research progress to all members of the research team, including collaborators at the Universities of Liverpool and Imperial College London. The researcher will provide regular, clear verbal and written progress reports to the research group leader (the Professor of Chemical Modelling). The researcher 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.  Postdoctoral research experience in computational chemistry or a related field.  Excellent computing skills.  Programming experience, including Python | Experience with use of, or development of, machine learning methods.  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 management of software development.  Experience with database management. | Application form, references, and interview |
| Planning and organising | Able to organise own research activities to deadline and quality standards.  Ability to balance multiple projects.  Proven ability to organise a range of high quality research activities to deadline and quality standards, ensuring plans complement broader research strategy |  | Application form, references, and 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  Able to apply originality in modifying existing approaches to solve problems |  | 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 | Strength at working proactively with colleagues in other institutions, contributing specialist knowledge to achieve project outcomes.  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. |  | 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 |  |  |  |