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**Job Description**

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| **Job title** | Research Associate in Machine Learning and Reaction Modelling |
| **Department/School** | Chemistry  |
| **Job family** | Education and Research |
| **Grade** | 7 |
| **Reporting to** | Dr Matthew Grayson (PI) |
| **Responsible for** | Day-to-day co-supervision of doctoral and/or undergraduate students  |
| **Location** | University of Bath premises  |

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| **Background and context** |
| We have an exciting opportunity funded by the EPSRC to work on the development of new synthesis prediction tools. You will join the Grayson group in the Department of Chemistry to develop fast, accurate and mechanism-based reactivity prediction models by combining machine learning with reaction modelling for applications in organic synthesis, covalent drug design and toxicology. To demonstrate their broad applicability, you will then apply the models to rationalising experimental reactivity data of organic and biological reactions for which the use of traditional modelling approaches would be prohibitively slow. |

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| **Job purpose** |
| To train and validate machine learning models that can correct energy barriers obtained from rapid molecular modelling techniques to those derived from prohibitively slow, high-accuracy methods. To demonstrate the broad utility of these models, they will then be used to rationalise experimental reactivity data of biologically and synthetically relevant systems for which the use of current modelling approaches would be prohibitively slow. |

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| **Main duties and responsibilities**  |
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| **1** | Conduct individual and/or collaborative research projects. Contribute to the design and execution of the project e.g. timetabling and meeting project milestones; participating in regular discussions with collaborative partners. Generate, collect and analyse existing data related to the project using qualitative and/or quantitative techniques. |
| **2** | Writing up results of research and contributing to the publication of results in high-quality peer-reviewed academic literature. |
| **3** | Disseminating results of research project as appropriate to the discipline through activities such as* overseas research visits
* conference presentations
* public engagement activities
 |
| **4** | Participate in departmental/group meetings and prepare and deliver presentations/seminars to project team, internal and external stakeholders or funders. |
| **5** | Assist with the supervision of postgraduate students and undergraduate project students and the assessment of student knowledge. |
| **6** | Continually update knowledge and understanding in field or specialism to inform research activity. |
| **7** | Identify sources of funding and provide assistance with preparing bids to funding bodies. Develop ability to secure own funding e.g. travel grants.  |
| **8** | Contribute to the development of research objectives and proposals for own or joint research projects, with assistance of a mentor, if required. |
| **9** | Disseminate knowledge of research advances to inform departmental teaching. |
|  | You will from time to time be required to undertake other duties of a similar nature as reasonably required by your line manager. You are required to follow all University policies and procedures at all times and take account of University guidance.  |

**![logo-uob-resize[1]]() Person Specification**

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| **Criteria** | **Essential** | **Desirable** |
| **Qualifications** |  |  |
| A PhD degree (or to be in the process of completing one) | ✓ |  |
| **Experience/Knowledge** |  |  |
| Postdoctoral research experience |  | ✓ |
| Experience in machine learning |  | ✓ |
| Experience in coding (any language) | ✓ |  |
| Experience in reaction modelling |  | ✓ |
| Demonstrated awareness of latest developments in the field of research | ✓ |  |
| Has published or has the potential to publish in high quality, peer reviewed journals | ✓ |  |
| **Skills** |  |  |
| Ability to conduct individual research work | ✓ |  |
| Ability to organise and prioritise own workload to meet required deadlines | ✓ |  |
| Ability to write research reports / publications | ✓ |  |
| Ability to disseminate research through both formal and informal presentations | ✓ |  |
| Excellent oral, interpersonal and written communication skills | ✓ |  |
| Proficiency in core IT skills | ✓ |  |
| **Attributes** |  |  |
| Commitment to working within professional and ethical codes of conduct | ✓ |  |
| Innovation and developing creative solutions | ✓ |  |
| Commitment to excellence in research | ✓ |  |
| Enthusiasm and self-motivation | ✓ |  |
| Tenacity – working to achieve own and team objectives and to overcome obstacles | ✓ |  |
| Ability to be an effective team worker | ✓ |  |
| Commitment to safe working practices | ✓ |  |