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**Job Description**

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| **Job title** | Research Associate |
| **Department/School** | Mathematics |
| **Job family** | Education and Research |
| **Grade** | 7 |
| **Reporting to** | Principal Investigator (PI) |
| **Responsible for** | Day to day supervision of other staff e.g. technical staff or co-supervision of doctoral or undergraduate students may be required. |
| **Location** | University of Bath premises |

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| **Background and context** |
| A UK-funded postdoctoral research position is available at the University of Bath to accelerate Kinetic Monte Carlo Methods for Novel Solar Cell Design. The position is funded by the EU Horizon2020 Project Energy Oriented Centre of Excellence, EoCoE, whose aim is to support numerical modelling of key technologies in sustainable energy sources. Bath is a node in the consortium and involved in the thematic area of "Materials for Energy” www.eocoe.eu/workpackages/materials-energy. This postdoc position will include strong interactions with the other nodes of the EoCoE consortium.  The aim of the project at Bath is a multiscale study of novel perovskite solar cell materials  https://www.electronicsweekly.com/news/research-news/perovskite-materials-solar-expert-speaks-2017-05/ and https://en.wikipedia.org/wiki/Perovskite\_solar\_cell  The EoCoE node at Bath is funded by additional EU and EPSRC grants and training networks to look at perovskite and battery materials and consists of the interdisciplinary team Prof Robert Scheichl in the Department of Mathematical Sciences, [www.maths.bath.ac.uk/~masrs](http://www.maths.bath.ac.uk/~masrs), and the computational scientists Prof Alison Walker. <http://people.bath.ac.uk/pysabw/>, and Prof Saiful Islam http://people.bath.ac.uk/msi20.    Kinetic Monte Carlo, KMC, methods are required to predict device behaviour from the material properties at the microscopic scale. The postdoc will work with Prof Robert Scheichl on replacing tried and trusted mathematical algorithms employed in KMC by newer methods with better scaling properties. |

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| **Job purpose** |
| Work funded by EoCoE so far has mainly focussed on atomistic studies of the microscopic processes, such as charge and exciton hopping, recombination rates and light absorption. In the remaining 16 months of the project, using the parameters obtained from the atomistic simulations, work will focus on kinetic Monte Carlo simulations at the mesoscale, computing current-voltage characteristics, charge mobilities and parameters for calculating recombination that can subsequently feed into faster device design offered by continuum models where current-voltage characteristics are obtained.  The kinetic Monte Carlo (KMC) method (http://people.bath.ac.uk/pysabw/abwmod.html, middle column) is closely related to the Gillespie algorithm (https://en.wikipedia.org/wiki/Gillespie\_algorithm). Walker is one of the leading researchers in the development and application of KMC. In line with the overarching work package WP1 of EoCoE, this project will focus on ‘reengineering’ the computationally intensive parts of KMC with a view of improving the overall performance and making them more suited to supercomputers with high concurrency. This is likely to involve replacing tried and trusted mathematical algorithms by newer methods with better scaling properties. In particular, we intend to investigate novel multilevel Monte Carlo ideas (http://epubs.siam.org/doi/abs/10.1137/130940761, https://arxiv.org/abs/1409.1838), as well as fast and massively parallel Poisson solvers for the modelling of long-range interactions. |

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| **Main duties and responsibilities** | |
|  | Responsible to the PI/CI for (as appropriate to discipline): |
| **1** | Conduct collaborative research projects. Take a lead in developing new codes and running existing codes. Interpret the results from the code in the light of other models and of experimental data available through the collaborations. |
| **2** | Writing up results of research and contributing to publishing of results in high-quality peer-reviewed academic literature. |
| **3** | Project management: e.g. timetabling and meeting project milestones; participating in regular discussions with collaborative partners. Liaise with key stakeholders/industrial partners and conduct focus groups. |
| **4** | Disseminating results of project e.g. by presentations at conferences, overseas research visits, public engagement activities. |
| **5** | Participate regularly in group meetings and prepare and deliver presentations to project team, internal and external stakeholders or funders. |
| **6** | Assist with the supervision of graduate students and undergraduate project students and the assessment of student knowledge. |
| **7** | Continually update knowledge and understanding in field or specialism to inform research activity. |
| **8** | Identify sources of funding and provide assistance with preparing bids to funding bodies. Contribute to securing of own funding e.g. travel grants. |
| **9** | Develop research objectives and proposals for own or joint research, with assistance of a mentor if required. |
| **10** | Disseminate knowledge of research advances to inform departmental teaching effort to the extent possible with teaching allocations. |

**Person Specification**

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| **Criteria** | **Essential** | **Desirable** |
| **Qualifications** |  |  |
| A PhD degree in subject area of direct relevance for the project and significant relevant experience where applicable. | √ |  |
| **Experience/Knowledge** |  |  |
| Demonstrated significant depth and breadth of specialist knowledge of subject matter to contribute to research programmes and to the development of departmental research activities. | √ |  |
| Demonstrated awareness of latest developments in the field of research and in research design | √ |  |
| Demonstrated potential to publish in high quality, peer reviewed journals | √ |  |
| **Skills** |  |  |
| Ability to prepare research proposals, to conduct individual research work and to disseminate results | √ |  |
| Ability to organise and prioritise own workload | √ |  |
| Ability to write research reports and to effectively disseminate outcomes | √ |  |
| Excellent oral, interpersonal and written communication skills | √ |  |
| Proficiency in IT skills | √ |  |
| **Attributes** |  |  |
| Commitment to working within professional and ethical codes of conduct | √ |  |
| Innovation and developing creative solutions | √ |  |
| Enthusiasm and self-motivation. | √ |  |
| Organisation – able to plan and deliver work to meet required deadlines | √ |  |
| Tenacity – working to achieve own and team objectives and to overcome obstacles | √ |  |
| Ability to be an effective team worker | √ |  |