Job Related Information

This document includes information about the role for which you are applying and the information you will need to provide with your application.

1. Role Details

<table>
<thead>
<tr>
<th>Vacancy reference</th>
<th>14121</th>
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<tbody>
<tr>
<td>Job title:</td>
<td>Post Doctoral Research Associate</td>
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<tr>
<td>Reports to:</td>
<td>Senior Lecturer</td>
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<tr>
<td>Salary:</td>
<td>£29,799 to £38,833</td>
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<td>Terms and conditions:</td>
<td>Research Staff</td>
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<tr>
<td>Grade</td>
<td>AC2</td>
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<tr>
<td>Duration of post:</td>
<td>24 months</td>
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<tr>
<td>Working hours:</td>
<td>Full-time</td>
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<tr>
<td>Location:</td>
<td>Milton Keynes</td>
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<td>Closing date:</td>
<td>Noon on 23 November 2017</td>
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<tr>
<td>Type of application form accepted:</td>
<td>Short</td>
</tr>
<tr>
<td>Number of referees required:</td>
<td>2</td>
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<tr>
<td>Unit recruitment contact:</td>
<td>Fiona McGavin</td>
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2. Summary of duties

This postdoctoral position is funded by the grant *R-matrix suites for multielectron attosecond dynamics in atoms and molecules irradiated by arbitrarily polarised light* (R-MADAM) supported by EPSRC as part of their Software as an Infrastructure strategy under a Software Flagship Project Call. This is a 2-year project involving The Open University and Queen’s University Belfast with collaborators from University College London, Max Born Institute for Non-linear Optics, Quanternol Ltd. and the Scientific Computing Department at STFC.

The main objective of the project is the development of software for the accurate description of atoms and molecular systems in intense, ultra-short light fields with arbitrary polarisation. This involves generalising and interfacing two world-leading suites of codes: the R-matrix with time-dependence codes (RMT) for ultra-fast atomic dynamics and the UKRmol+ suite for electron/positron scattering and photoionisation processes in molecules. The UKRmol+ suite (http://ccpforge.cse.rl.ac.uk/gf/project/ukrmol-in/) is a very widely used time-independent package for studying electron-molecule collisions. Recent major improvements in algorithms and extensions to its functionality have improved our ability to treat electron scattering from complex molecules and enabled us to produce data essential for the study of laser induced processes in small molecules. Currently, the integral evaluation, Hamiltonian build and diagonalization steps in the suite are parallelized. However, the calculation of dipole transition moments needed for photoionization studies relies on the serial diagonalization of the Hamiltonian for each required symmetry. Significant efficiencies can be achieved if this calculation is parallelized. In addition, the routines involved in the generation of configuration state functions necessary to build the Hamiltonian are inefficient and lacking in flexibility.

The PDRA will undertake the redevelopment of those parts of the UKRmol+ suite of codes that deal with the evaluation of dipole transition moments and the generation of configuration state functions. Specifically, they will: (i) integrate within the Hamiltonian construction/diagonalisation step (and therefore parallelise) the evaluation of transition moments between bound and continuum states needed to study laser-molecule interactions; (ii) develop procedures and routines to generate configuration state functions (CSF) in a highly selective way tuned for the continua of molecules and thus ensure the suite produces input data of sufficient quality for the RMT suite and other software describing attosecond physics. The PDRA will also contribute to disseminating the new suites to current and potential new users by helping in the organization of a workshop, attending meetings, giving presentations and writing papers.

3. Person specification

Requirements  (E = Essential/ D = Desirable)

<table>
<thead>
<tr>
<th>Education, qualifications and training</th>
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<tr>
<td>Successful completion (or near completion) of a PhD in physics, computational chemistry or a related subject.</td>
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<table>
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<tr>
<th>Knowledge, work and other relevant experience</th>
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<tr>
<td><strong>Essential:</strong></td>
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<tr>
<td>• Experience of applying techniques of high performance computing to problems in physics/chemistry</td>
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<td>• Excellent knowledge of Fortran 95</td>
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<td>• Experience of developing large scale computer programs, especially those involving parallelism</td>
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<td>• Good numerical analysis skills</td>
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- Experience of working using a Unix-based operating system

**Desirable:**
- Knowledge of Fortran 2003
- Knowledge of MPI and OpenMP parallel programming protocols
- Experience in developing, programming, documenting and testing scientific software
- Experience using version control software (subversion, Git, or the like)
- Familiarity with numerical libraries (e.g. lapack, scalapack)

### Personal abilities and qualities

**Essential:**
- Ability to work independently and cooperatively as a productive member of a geographically distributed team
- Problem-solving ability
- Ability to manage workload and deliver results to an agreed schedule

**Desirable:**
- Experience working on collaborative code development projects
- Well-developed verbal communication skills
- Good technical writing skills

4. **Role specific requirements e.g. Shift working**

The project involves close collaboration between researchers at The Open University and Queen’s University Belfast working under the same grant. It is expected that both PDRAs employed by the grant will travel with some regularity between Belfast and Milton Keynes to discuss and plan code development.

5. **About the unit/department**

**Faculty of Science, Technology, Engineering & Mathematics**
The newly formed Faculty of Science, Technology, Engineering and Mathematics (STEM) comprises:

- School of Computing & Communications
- School of Environment, Earth & Ecosystem Sciences
- School of Engineering & Innovation
- School of Life, Health & Chemical Sciences
- School of Mathematics & Statistics
- School of Physical Sciences
- Knowledge Media Institute
- Deanery including teams supporting Curriculum, Research and Enterprise, Laboratory Infrastructure and Faculty Administration

“We aspire to be world leaders in inclusive, innovative and high impact STEM teaching and research, equipping learners, employers and society with the capabilities to meet tomorrow’s challenges”

The Faculty of STEM consists of 700 staff and 1,800 Associate Lecturers. The Faculty delivers over 185 modules across undergraduate and postgraduate curriculum, supporting more than 20,000 students (full time equivalents) which is 29% of the OU total.

The Faculty generates more research income (circa £20M) than any other Faculty in the University, supported by a comprehensive laboratory infrastructure.

We are proud of our distinctive values and capabilities underpinning our aspiration:
We are inclusive:
- We transform people’s lives, ensuring STEM education is openly accessible to many thousands of students from diverse backgrounds – our students express high satisfaction with their study experience
- We engage the public in exciting citizen science and engineering, including through free open educational resources, multi-platform broadcasting, outreach to inspire the next generation and with programmes to encourage more women into STEM

We are highly innovative:
- We are at the forefront of innovative developments in teaching practical science and engineering at a distance, through simulated and remote access laboratories and practical experimentation
- Our high quality teaching and curriculum are informed by world-leading research, strong links with professional bodies and communities of practitioners, as well as by scholarship focused on continuously improving our STEM pedagogy

We deliver significant social and economic impact:
- We provide STEM higher education at a scale and reach unsurpassed in the UK, with a sizeable international reach and further growth potential
- We inject transferable STEM skills and knowledge direct into the workplace for immediate employee and employer benefit, as students combine study while working
- The employability value of our courses is underpinned by accreditation from leading STEM Professional Bodies and Learned Societies, as well as partnerships and sponsorship with leading employers
- Our high quality, applied and academically relevant teaching and research addresses real-world issues, delivering impact for industry and society, including addressing pressing STEM skill shortages across the UK

School of Physical Sciences
The School of Physical Sciences is a lively and innovative community of approximately 80 academic and research staff and 70 PhD students, mostly based in Milton Keynes. Our curriculum is supported by associate lecturer staff based all over the UK and Ireland; physics, astronomy and planetary sciences undergraduate modules are currently being studied by hundreds of students all over the world and we also contribute to an introductory and interdisciplinary science modules being studied by several thousand students.

Our research covers a wide range of subjects, broadly aligned with the research disciplines of
- Astronomy
- Physics
- Planetary and Space Sciences
- Space Instrumentation
- Physics Education

We have an unparalleled suite of analytical instrumentation in our modern laboratories on campus; this is complemented by our regular use of multi-national facilities such as the Diamond synchrotron and ESO’s telescopes. We have contributed to well-known space missions such as the Rosetta Mission, and have developed some of our spaceflight instrumentation for medical and environmental applications.

School members also contribute to the Open University’s teaching on a large range of modules and we have been at the forefront of many innovations in distance education, including the OpenScience Lab. We are members of SEPnet, the South East Physics Network. Our commitment to equality and diversity has been recognised by the award of “Juno Champion” status by the Institute of Physics and an Athena SWAN Silver Award.

We currently offer undergraduate qualifications in Mathematics and Physics and Natural Sciences (with a physics pathway and an astronomy and planetary science pathway), with a strand which carries Institute of Physics accreditation. We are in the process of refreshing the curriculum, both at entry level to reflect the diverse range of entry qualifications of our students, and at Stage 3. In the near future we are likely to offer a BSc (Hons) Physics and/or a BSc (Hons) Astronomy and Planetary Science and/or an integrated MPhys,
including physics, astronomy, planetary and Space science. A new MSc in Space Science and Technology is currently recruiting students and will run for the first time from February 2017.

**Priority Research Areas in the School of Physical Sciences**

**Astronomy**
- The Compositional Universe: exploiting the spectroscopic discovery space from ALMA, JWST, SPICA, SOFIA and IRAM/NOEMA, E-ELT, VLT, SKA, JCMT, SALT, LOFAR, ELIPS, Herschel, SDSS-IV, Euclid strong lensing, etc., to study galactic star formation, evaporating exoplanets, and the physics of galaxies in the distant universe. We will further develop our laboratory/observational astrochemistry research to focus on the development of molecular compositional diagnostics.
- The Time-Domain Universe: exploiting the discovery space of new and future telescopes e.g. Gaia, LIGO, PLATO 2.0, TWINKLE, VLT and LSST, in studies such as galactic and extragalactic stellar populations using leading follow-up facilities such as SALT, or (as part of a wider follow-up network) our robotic telescopes, with a focus on key processes such as stellar binarity.

**Physics**
- Biomedical physics: to understand physical phenomena involved in conditions such as cancer and cardiovascular diseases and their treatment through experimental and theoretical investigations of a range of approaches such as electron-driven processes in radiation treatment and imaging, use of nanoparticles for cancer therapy and plasma sources for biomedical purposes.
- Quantum correlated systems: theoretical and experimental study of quantum correlations in atomic, molecular and condensed matter systems, and the development of practical applications such as quantum enhanced devices and the functionalisation of materials, as well as the development of multi-purpose software to treat electronic continua.
- Engineering physics: applied plasma research aimed at developing novel functional materials, understanding electron induced processes in nanofabrication and the development of plasma-driven techniques for advanced materials applications.

**Planetary and Space Science**
- Application of advanced analytical techniques, laboratory simulation, remote observation and modelling to investigate the key processes involved in the formation and evolution of the Solar System and the planetary bodies it contains, including the search for habitable environments and the presence of life.
- Maintain and build high scientific credibility for our analytical expertise by exploiting the performance of existing instruments and updating the analytical infrastructure in order to secure leading involvement in upcoming sample-return missions, and maintain access to the most important planetary samples. Particular strengths are in the measurement of light-stable isotopes using conventional mass spectrometry and *in-situ* analysis of samples.
- Development and expansion of our expertise in planetary environments using modelling, remote sensing and the use of field analogues and simulation facilities on Earth, and secure further leading science team involvements in future planetary space missions.

**Space Instrumentation**
- Development of imaging sensors and instruments for space applications, with expertise in a range of wavelengths from IR to X-ray and the study of the effects of radiation damage, in order to secure involvement in future space missions.
- Development of miniaturized analytical instrument systems for planetary exploration missions, particularly for the measurement of volatiles, organic materials and their light stable isotope composition, and securing leading involvement in future planetary exploration missions.
- Knowledge exchange between the UK technology industry and academia, utilising the technologies and expertise in detectors and mass spectrometer systems to provide commercial products and solutions.

**Physics Education Research**
- Remote and virtual experimentation
- Concept inventories
- Interactive online assessment
- Demographic differences in achievement
6. How to obtain more information about the role or application process

If you would like to discuss the particulars of this role before making an application please contact Jimena Gorfinkiel on +44 (0)1908 858205 or email: Jimena.Gorfinkiel@open.ac.uk.

If you have any questions regarding the application process please contact Fiona McGavin on 01908 858110 or email: STEM-Recruitment@open.ac.uk.

7. The application process and where to send completed applications

| Your application should contain: | Short Application Form  
| CV  |
| Please ensure that your application reaches the University by: | Noon on 23 November 2017  
| E-mail your application to: | STEM-Recruitment@open.ac.uk  
| Or post it to Name/Job title: | Fiona McGavin, Staffing Adviser  
| Department/Unit: | Deanery, Faculty of Science, Technology, Engineering & Mathematics  
| Address: | The Open University, Walton Hall, Milton Keynes, MK7 6AA |

8. Selection process and date of interview

| The interview panel will be chaired by: | Dr Jimena Gorfinkiel  
| The other members of the interview panel will be: | Dr Sam Eden  
| The interviews will take place on: | Early December  
| The selection process for this post will include | A 30-45 minute interview. The candidate will be asked to spend the first 5-10 minutes highlighting his/her past experience in software development.  

We will let you know as soon as possible after the closing date whether you have been shortlisted for interview. Further details on the selection process will also be sent to shortlisted candidates. Applications received after the closing date will not be accepted.