Research Associate in Computational And Theoretical Photochemistry

1 JOB DESCRIPTION

Faculty / School or Division: School of Chemistry

Faculty/School or Division Address: Cantock's Close, University of Bristol, BS8 1TS

Job Family:	**Research and Teaching**		
Grade/Pathway:	Grade I	**Salary range:**	£40,704 - £45,641 per annum
Hours of work:	35 hours / week	**Contract type:**	Open ended
Work pattern:	Full time	**Vacancy Reference Number:** ACAD108772	

1.1 Main Job Purpose

A postdoctoral research position in computational and theoretical photochemistry is available in the School of Chemistry at the University of Bristol, supported by the ERC Consolidator Grant 101229789 **In Silico Photochemistry of Atmospheric Molecules in Aqueous Aerosols** (ISPAMIA). The project is led by Prof Basile Curchod (University of Bristol, UK).

This project will investigate the photochemistry of atmospheric volatile organic compounds (VOCs) at the air-water interface and in aqueous aerosols. The project will comprise (1) theoretical developments to describe the complex environment created by an aqueous aerosol, from an electronic structure and nuclear dynamics perspective, and (2) the application of these methods to simulate the unimolecular and bimolecular photochemistry of selected VOCs in and at the air-water interface of an aqueous aerosol. This project builds on recent work by our research group on studying the gas-phase photochemistry of atmospheric and complex molecules (e.g., Refs. [1-5]).

The theoretical developments will be implemented in the open-source codes OpenFMS and ABIN. The simulations of VOCs at the air-water interface and in the aqueous aerosol will use machine-learned potentials to accelerate the sampling of ground-state distributions representative of the VOC in different environments. These ground-state distributions will then be used to predict photolysis rate coefficients for the air-water interface and the bulk of the aqueous aerosol. Enhanced sampling strategies will be used to simulate the bimolecular reactivity of VOCs in their triplet state in the bulk of the aerosol or at the air-water interface. The present postdoctoral position will focus on the study of the interaction of selected VOCs with different models of the air-water interface of an aqueous droplet.

Further details of the In Silico Photochemistry Group can be found at www.in-silico-photochem.com, where a list of the group's publications can be found as well.

[1] J. P. Figueira Nunes *et al*, J. Am. Chem. Soc., **146**, 4134 (2024). https://doi.org/10.1021/jacs.3c13046
[2] A. Prlj *et al*, J. Phys. Chem. Lett., **11**, 5418 (2020). https://doi.org/10.1021/acs.jpclett.0c01439
[3] J. Janoš *et al*, J. Chem. Phys., **160**, 144305 (2024). https://doi.org/10.1063/5.0203105
[4] C. Clarke *et al*, Nat. Commun., **13**, 937 (2022). https://doi.org/10.1038/s41467-022-28582-4
[5] E. M. Burrow *et al*, J. Am. Chem. Soc*.*, **147**, 36987 (2025). https://doi.org/10.1021/jacs.5c13075

The successful applicant will join the School of Chemistry, which is one of the very best Chemistry departments in the UK. In the latest Research Excellence Framework (REF 2021), the School was ranked 1st out of 41 Chemistry departments based on the assessed categories of Outputs, Impact and Environment. The School is located within the Faculty of Science and Engineering, which is one of the top-ranked science and engineering faculties in the UK. Currently, the School has an academic base comprising around 60 academic staff, approximately 80 postdoctoral researchers, 200+ postgraduates and about 650 undergraduates. The School's research and teaching are supported by about 30 technical staff, and departmentally based administrative support is provided by a further 20 staff.

1.2 Main Statement of Responsibilities

Research Responsibilities

- Train machine-learned potentials for atmospheric VOCs and their interaction with water in different environments (bulk, air-water interface).
- Build different models of the air-water interface (with various components, e.g., ions).
- Study the ground-state distribution of a VOC at the air-water interface using different molecular dynamics approaches (ab initio molecular dynamics, quantum-thermostated dynamics, path-integral molecular dynamics).
- Analyze and interpret these theoretical simulations in detail.
- Calculate experimental observables (photoabsorption cross-sections) in direct collaboration with project collaborators.
- Benchmark electronic-structure methods to describe excited electronic states of the VOC surrounded by water molecules.
- Collaborate with other members of the ISPAMIA Team to prepare excited-state dynamics simulations.
- Contribute to the maintenance of the group servers and workstations.
- Prepare results from calculations for publication, and write draft manuscripts.
- Contribute to the supervision of graduate students and undergraduate project students undertaking research in the group of Prof Basile Curchod.
- Contribute more widely to the Physical and Theoretical Chemistry section within the School of Chemistry, by attending and contributing to group meetings and seminars.
- Collaborate with project co-investigators at other UK universities, including ultrafast spectroscopists and theoretical chemists.

Administration Responsibilities

- Contribute to the writing of publications for dissemination of the research in the scientific literature.
- Participate in regular meetings with collaborators on the ERC-funded project.
- Contribute to the website of the research programme.

- Present research outcomes in seminars and at national and international conferences.
- Supervise postgraduate and undergraduate students.
- Contribute to outreach activities.
- Engage effectively in the University's Staff Review and Development process and develop, with advice, an awareness of their own professional development needs and a personal development strategy, engaging with continuing professional development appropriate to the role.
- Consistently act as a good citizen, actively participating in the daily working life of the School of Chemistry.
- Undertake relevant training and development activities to develop capacity for taking on wider responsibilities (including small amounts of teaching) and to support their career development.
- Maintain academic standards and freedom, and work in accordance with University policies (e.g. equal opportunities, ethics and health and safety policies).

Teaching Responsibilities

As this role is a Pathway 2 (Research) role, there are no formally specified teaching duties required of the role-holder. However, other commitments permitting, the role-holder may be given development opportunities to undertake activities such as teaching on Masters and Doctoral programmes and/ or supervising MSc dissertations within the School of Chemistry, as appropriate.

1.3 Relationships

Line manager: Prof Basile Curchod

Line manager to (where appropriate): Not applicable

1.4 Job Hazards/Safety Critical Duties (Pre-employment health screening)

Not applicable

---

2 PERSON SPECIFICATION

2.1 Relevant Experience, Skills and Knowledge

Essential

- Experience in theoretical/computational chemistry applied to atmospheric chemistry.
- Experience in using classical molecular dynamics or ab initio molecular dynamics.

- Experience in describing complex environments in calculations/simulations.
- Practical experience with different software packages for molecular dynamics and electronic structure theory.
- Experience with coding and scripting for data analysis.
- Preparation of manuscripts for publication.
- Ability to organise their own time and work effectively, to meet deadlines and manage competing priorities.

Desirable

- Experience in training machine-learned potentials.
- Experience in using path-integral molecular dynamics.
- Experience with electronic-structure methods beyond the ground state and benchmarking.
- Experience with compiling codes and using different computational architectures.
- Demonstrable ability to collaborate with experimental groups.

2.2 Relevant Qualifications

Essential

- A PhD in Physical Chemistry, Chemical Physics or Physics or near completion, or equivalent research experience in an academic, industrial or clinical setting equivalent to a PhD**.**
- A good honours degree (or equivalent) with subject knowledge in Chemistry, Chemical Physics or Physics.

2.3 Communication and Interpersonal Skills

Essential

- Ability to communicate complex information clearly and accurately in English, both in written and oral forms.
- Ability to lead in the preparation of manuscripts for publication and communicate the outcomes of the project to researchers from a broad range of disciplines.

Desirable

- Experience in giving oral and poster presentations at research conferences or within a department.
- Experience in writing scientific papers.
- Necessary skills to assist in the supervision of graduate students and undergraduate project students.

3 CAREER PATHWAY AND OTHER RELEVANT INFORMATION

3.1 Career Pathways

All members of academic staff have a clear career pathway involving a series of levels with distinct role profiles, each with its unique requirements. Each profile sets out what is expected of an academic at the particular level. The role profiles also set out a collection of competencies expected for each level. Promotion to the next level may occur after these competencies have been attained in conjunction with the expectations outlined in the Promotions Process and Academic Promotions Framework (APF) applicable to the role. .

The academic pathways are as follows:

Career Pathway One - academic roles that combine teaching, research and administrative duties.

Career Pathway Two - academic roles focusing on research and associated administrative duties.

Career Pathway Three – academic roles focusing on teaching and associated administrative pathways

This post is located on Pathway Two. Role Summaries setting out what is expected of an academic at each particular profile level on pathway two can be found below. Please note that an appointment may be made at any level of the pathway.

A schematic diagram of the career pathways can be found at http://www.bristol.ac.uk/hr/grading/academic/.

The University has two procedures for promotions depending on the level of promotion being applied for as follows:

Promotion up to Senior Lecturer / Senior Research Fellow
Promotion to Associate Professor or Professor

The procedure for Promotion up to Senior Lecturer / Senior Research Fellow describes the process for anyone on the academic career pathways and is based on the concept of readiness as determined with managers using the Academic Promotions Framework (APF). Eligibility for making a case for promotion is subject to:

1. Having a contractual expectation and meeting the performance requirements described in the Promotion up to Senior Lecturer / Senior Research Fellow process
2. Completion of a full year of service following appointment and successful completion of their Initial Service Review (ISR)
3. Meeting the expectations set out in the CREATE policy for those with teaching responsibilities (pathway 1 and 3), e.g. those seeking promotion to Senior Lecturer should achieve and have been formally notified of their Fellowship (ratified outcome) through the University's CREATE scheme before applying

The procedure for Promotion to Professor covers staff for promotion to profile level d2 (Associate Professor) and profile level e (Professor) on all pathways in the Academic Career Pathway framework.

3.1.1 Role Summaries

Research Associate (Level a)
Role holders at this level are concerned with *assisting* an individual research leader or team to conduct a particular study (or group of studies). They will generally be involved in data generation and/or collection using standard and well-defined methods developed by others. They will be working under close supervision by, and direction from, a more senior researcher, who will be ultimately responsible for the project. This may be the entry level for some staff who are expected to train and/or develop to take on more senior researcher roles. Role holders will be provided with academic and pastoral support within the department (including counselling on realistic career opportunities) and training will be available designed to develop their competences and to prepare them to take on more responsibilities associated with a higher grade.

Senior Research Associate (Level b)
Role holders at this level will be experienced and professional researchers (or have considerable professional experience) and will be specialists in a particular area or methodology, drawing upon knowledge gained from postgraduate research and/or working within a Level a role. They will be *associated* with a particular project (or projects) and will contribute ideas, and/or enhancement of techniques or methodologies. They will be expected to do some writing for dissemination outside the Department. They will still be working under supervision, but will be expected to take significant initiatives in their work and consult with the Principal Investigator over the details of the project. They may, where practical, contribute to the department's teaching, through supervision of projects, overseeing practical classes, or taking small group classes. They will be provided with academic and pastoral support within the department and training will be available designed to develop their competences (including counselling on realistic career opportunities) and prepare them to take on more responsibilities associated with a higher grade.

Research Fellow (Level c)
Role holders at this level will have substantial experience of research (normally not less than six years). They will initiate and take responsibility for some research projects and may be Principal Investigators or, where a Research Council does not permit this, act as though they were Principal Investigators. They will be involved in administration relevant to their projects (e.g. helping to prepare bids for research funding), managing other researchers and monitoring research budgets. They will be expected to be undertaking research individually and/or collectively and to be advancing the state of knowledge and understanding within their particular area of expertise. They will be publishing regularly in high quality outlets. They are likely to provide some teaching support for the department (consonant with the terms of their funding). They will be expected to be establishing a growing reputation within their particular research field and academic discipline and to be developing and demonstrating intellectual independence.

Senior Research Fellow (Level d)
Role holders at this level will have extensive experience in research and research management. They will normally be Principal Investigators, leading collaborative research bids and research teams, or driving forward innovative research themselves. They will be involved in scholastic projects (e.g. editing journals and academic books), and be making a significant leadership and/or management

contribution within their department or the wider university, to be participating in national/international academic networks and conferences. They may be transferring their knowledge through some teaching and/or supervision to undergraduate or graduate students (consonant with the terms of their funding). Role holders at this level will be independent researchers and will have an established national and growing international reputation within their academic discipline generally and research field in particular.

Professorial Research Fellow (Level e)

Role holders at this level will have very extensive experience of research leadership and related management/administration. They will enjoy a wide recognition for their expertise within the academic community internationally (as evidenced by conference invitations, journal editorships, office holding in specialist groupings, associations with appropriate Research Councils etc.). They will have made recognised and significant contributions to the developing knowledge and understanding of their research area. They will already have responsibilities for the creation, initiation, development and overall management of significant research programmes. They will 'profess' their discipline within the Department, as appropriate and consonant with the terms of their funding. They may also carry significant leadership roles within the Faculty or University.

3.2 Additional Statistical Information. This can also include any other relevant contextual or specific role or team information not included elsewhere

3.3 Relevant Physical and Environmental Information

3.4 Key Contacts

Contact Type	Purpose of Contact
• Prof Basile Curchod	Progress on the research project
• Other research associates	Sharing the research facilities
• Postgraduate students	Sharing the research facilities
• Undergraduate project students	Training & supervision
• School of Chemistry technical staff	Support for research