UNIVERSITY COLLEGE LONDON

Job Description

Job Title: Research Associate
Department: Chemistry
Location: UCL Bloomsbury Campus
Reports to Richard Catlow
Grade: 7

The Project
The project “Transition metal controlled nitrogen chemistry in zeolite and protein environments using a unified quantum embedding model”, funded by EPSRC (EP/R001847/1), is undertaken in collaboration with the team of Tom Keal at STFC Daresbury Laboratory, leading overall code developments and life science applications, and our group focusing on development and implementation of new approaches to modelling spectroscopic signatures and reactivity of heterogeneous catalysts.

Main Purpose
The postholder will be required to develop and implement theoretical models for spectroscopic signals of active centres and reactants in heterogeneous catalysts and proteins. The new tools developed within the computational chemistry ChemShell code will be extensively validated against experimental data from our collaborator Andrew Beale at the Harwell Research Hub. Our objectives are:

- To calculate vibrational, UV-vis and X-ray absorption spectroscopic signatures for Cu-containing zeolites to establish the nature of the Cu active sites.
- To determine mechanisms for the formation and reaction of ammonium nitrite-like complexes during the Selective Catalytic Reduction (SCR) reaction including solvent and thermal vibrational effects.

We will use both conventional QM/MM calculations and the advanced embedding model developed under the EPSRC “Scalable Quantum Chemistry with Flexible Embedding” project, which was motivated by limitations in quantum embedding methods for ionic materials. This includes a frozen density description of the cluster surroundings, which tackles the electrostatic anisotropy and spin polarisation of the environment, and describes solvent molecules quantum mechanically, without the computational cost of a full QM calculation. We will extend our model in a number of significant ways, including extending the frozen density treatment to covalent systems in order to enable calculations on both zeolites and proteins; developing methods for vibrational frequency calculations that can span both the full QM and frozen density regions, with anharmonic corrections for increased fidelity to experiment; extending frozen density embedding (FDE) to excited states through modifications to the kernel in TDDFT, enabling UV-visible spectroscopy in the FDE environment; and calculation of free energies in solvated environments through a QM/MM free energy perturbation approach. This will result in a unified, flexible embedding model for both solid state and biomolecular modelling with wide applicability to QM/MM simulations in general.

Last update: 10/8/2017
Introduction to UCL

UCL is one of the world's top universities. Based in the heart of London, it is a modern, diverse, outward-looking institution. At its establishment in 1826, UCL was radical and responsive to the needs of society, and this ethos – that excellence should go hand-in-hand with enriching society – continues today. UCL’s excellence extends across all academic disciplines; from one of Europe's largest and most productive hubs for biomedical science interacting with several leading London hospitals, to world-renowned centres for architecture (UCL Bartlett) and fine art (UCL Slade School).

UCL is a truly international community. Over 38,000 students study at UCL, of whom over 34% come from 140 countries outside the UK. Of our 12,500 staff, nearly one-third are also international. UCL offers more than 200 undergraduate programmes and more than 400 taught postgraduate programmes. Approximately 54% of the student community is engaged in graduate studies, with about 29% of these graduate students pursuing research degrees.

UCL's staff and former students have included 29 Nobel prize winners.

UCL is independently ranked as the most productive research university in Europe (SIR). It has the highest number of professors in any university in the UK (983) – and the best academic to student ratio of any UK university (The Times, 2014), enabling small class sizes and outstanding individual support.

In Research Excellence Framework 2014 (REF2014), UCL was rated the top university in the UK for 'research power'. It was rated top not only in the overall results, but in each of the assessed components: publications and other research outputs; research environment; and research impact. REF2014 confirmed UCL’s multidisciplinary research strength, with many leading performances across subject areas ranging from biomedicine, science and engineering and the built environment to laws, social sciences and arts and humanities.

Equality, Diversity and Inclusion

UCL was founded on the ethos of equality and diversity and was the first university in England to admit women on an equal basis to men. We are committed to fostering a positive cultural climate where all staff and students can flourish. UCL is a place where people can be authentic and their unique perspectives, experiences and skills seen as a valuable asset to the institution.

Some highlights below:

- **Race Equality Charter** - UCL is one of only eight universities in the UK to hold a Bronze Race Equality Charter award, recognising UCL's commitment to improving the representation, progression and success of minority ethnic staff and students.

- **Athena SWAN** - UCL holds an institutional Silver Athena SWAN award – this recognises our commitment to and impact in addressing gender equality. Departments at UCL are also engaged in the Athena SWAN charter, with 33 departments holding an award. UCL is the only university in the UK to be awarded both a Race Charter and Athena SWAN institutional Silver award.

- **Staff networks** - We have a number of staff networks that run a range of social, mentoring and development activities, for example Out@UCL (for LGBT+ staff) Parents and Carers Together (PACT) Enable@UCL (for Disabled staff), Racematters@UCL (for black and minority ethnic staff) Astrea women’s network and UCL Women

- **Sabbatical Leave following maternity** – UCL provides one term of sabbatical leave without teaching commitments for research-active academics returning from maternity, additional paternity, adoption or long-
term carer's leave. This support for returners enables staff to more quickly re-establish their research activity.

- **Encouraging flexibility** - 88% of respondents to the most recent UCL staff survey felt that their working time could be flexible. UCL's Work Life Balance policy gives employees the right to request a flexible working pattern.

Please see our [Equalities and Diversity Strategy 2015-2020](https://www.ucl.ac.uk/strategy) for information on our current priorities.

**Location and working environment**

UCL is a welcoming, inclusive university situated at the heart of one of the world's greatest cities. The Department of Chemistry operates from the main Bloomsbury Campus.

Find out more at [http://www.ucl.ac.uk/](http://www.ucl.ac.uk/)

**The Chemistry Department**

The Chemistry Department at University College London is the oldest in England, and today is one of the best in the UK, being ranked 2nd in the UK for the world-class impact of its research in REF(2014). We are located in Bloomsbury, at the heart of London, and offer an exciting and vibrant environment in which to study in one of the UK's top universities. The Department of Chemistry at UCL is committed to supporting excellence in both research and teaching. The department offers undergraduate BSc and MSci programmes in Chemistry and currently teaches 400 undergraduates registered in Chemistry as well as students who select Chemistry on the Natural Sciences programme and first year Chemistry for life scientists. The department also offers a number of Postgraduate Taught Masters courses with about 60 students per year and has an overall PGR student school of about 250 students.

The Chemistry Department has over 50 members of academic staff carrying out world-leading research. We specialise in the areas of organic synthesis, chemical biology, computational chemistry, nanotechnology, inorganic and materials chemistry, physical chemistry and chemical physics. The department has an annual research income of around £15 million, derived from many sources including the Research Councils (EPSRC, BBSRC, MRC, and NERC), European Commission and a wide range of charities and industrial partners in the UK, Europe and the USA.

Details about our research can be found on the departmental website [http://www.ucl.ac.uk/chemistry](http://www.ucl.ac.uk/chemistry).
Duties and Responsibilities

- To contribute to the methodological development and design and implementation of the embedding software. To take part in the application of the new methods under development to problems in heterogeneous catalysis and related topics.
- To present results of the development and applications to the scientific community in the form of papers submitted to peer reviewed journals, posters and talks given at scientific conferences.
- To prepare progress reports on research for funding bodies required for the progress of project.
- To contribute to the preparation and drafting of research bids and proposals as required for the progress of project.
- To contribute to the overall activities of the research team and department as required.
- To undertake a limited amount of teaching in relation to subject area within the expertise of the post holder.
- To contribute to the induction and direction of other research staff and students as requested within the expertise of the post holder.
- Responsible for ensuring that equipment is safe and maintained in working order.
- The job description reflects the present requirements of the post, and as duties and responsibilities change/develop, the job description will be reviewed and be subject to amendment in consultation with the post-holder.
- The postholder will carry out any other duties as are within the scope, spirit and purpose of the job as requested by the line manager.
- The postholder will actively follow UCL policies including Equal Opportunities and be expected to give consideration within their role as to how they can actively advance equality of opportunity and good relations between people who share a relevant protected characteristic and people who do not share it.
- The postholder will maintain an awareness and observation of Fire and Health & Safety Regulations.
- To be aware of and act upon:
  Disciplinary procedure and Disciplinary rules
  Grievance procedure
  Section 7 and 8 of the Health and Safety at Work Act
UNIVERSITY COLLEGE LONDON
Department of Chemistry

Person Specification for the Post of Research Associate

The applicant is required to submit with their application a cover letter detailing how they satisfy the Person Specification requirements below.

Essential Qualifications in relevant subject area
- Undergraduate Degree: Physics, Chemistry, Mathematics, Materials Science, or Engineering
- PhD: Theoretical, Mathematical or Computational Physics, Chemistry, or Materials Science, or Applied Mathematics, or Chemical Engineering
- GSCE English Grade C or above (or equivalent, e.g. IELTS)

Required Background for applicants from Natural Sciences (Essential)
- Appropriate undergraduate level Mathematics including Calculus and Linear Algebra
- Solid State Physics and / or Chemistry
- Foundations of Classical Mechanics, Electrostatics, Quantum Mechanics and Statistical Physics
- Molecular / Atomistic Modelling including Methods of Quantum Chemistry and Interatomic Potentials
- Programming languages used in the project (Fortran 2003 and Python)
- Unix/Linux scripting
- Track record of scientific software development

Required Background for applicants from Applied Mathematics (Essential)
- Appropriate undergraduate level Mathematics including Mathematical Analysis, Linear Algebra and Differential Equations, Methods of Mathematical Physics
- Foundations of Classical Mechanics, Electrostatics, Quantum Mechanics and Statistical Physics
- Molecular / Atomistic Modelling / Simulations Techniques
- Numerical methods including Linear Algebra and Optimisation and Discrete Mathematics
- Programming languages used in the project (Fortran 2003 and Python)
- Unix/Linux scripting
- Track record of scientific software development

Desirable Proficient Knowledge
- Numerical Methods in Mathematics including Linear Algebra and Optimisation
- Solid State Theory, Chemical Thermodynamics and Kinetics, Models of Solvation, Theory of Chemical Reactions
- Many-Electron Theory, Ab initio and Density Functional Theories for molecules and solids
- Embedded Cluster and Hybrid QM/MM techniques
- Frozen Density Embedding approaches
- Experience of software development in computational chemistry codes (especially ChemShell, NWChem, GAMESS-UK, LSDalton, GULP or DL_POLY)
- Parallel programming experience, using e.g. MPI or Global Arrays

Essential Skills
- Proven research skills, ability to analyse and write up data as evidenced by publications in peer reviewed scientific press
- Ability to present complex information effectively to a range of audiences as evidenced by presentations given in the form of talks and / or posters at scientific events
- Working mathematical skills with the ability to derive necessary mathematical expressions on paper and choose appropriate numerical techniques supported by evidence on record (thesis, papers, reports, etc.)
- Working skills for problem solving and creation of algorithms for computer implementation
Working command of (1) modern Fortran and (2) Python evidenced by independent stand-alone codes or excerpts from a larger package (>2,000 lines or equivalent). The evidence for each language may come from two separate codes or a single mixed-language code.

Essential Experience
- Experience of working in a research environment (university or research laboratory, etc.)

Essential Personal Qualities
- Commitment to high quality research
- Ability to collaborate, work as part of a team

Terms & Conditions of Employment
The post is a UCL grade 7 post, the salary for which ranges from £34,635 to £41,864 per annum (including London Allowance of £3,031 p.a.). Starting salary will be within this range depending on work experience. Please note, appointment at Grade 7 is dependent upon having been awarded a PhD; if this is not the case, initial appointment will be at Research Assistant Grade 6B (salary £30,316 to £31,967 per annum, including London Allowance of £3,031) with payment at Grade 7 being backdated to the date of final submission of the PhD thesis.

Progression through the salary scale is incremental. Cost of living pay awards are negotiated nationally and are normally effective from 1st August each year. UCL’s non-clinical pay and grading structure is at http://www.ucl.ac.uk/hr/salary_scales/final_grades.php.

UCL’s terms & conditions for research staff are at http://www.ucl.ac.uk/hr/salary_scales/Support_Research_tcs.php

The full range of benefits is at http://www.ucl.ac.uk/hr/benefits/employee_benefits.php

Equal Opportunities

www.ucl.ac.uk/hr/docs/equal_opportunity.pdf

The Department has been awarded a Bronze Athena Swan Award and we support the Athena beliefs that:

- The advancement of science, engineering and technology (SET) is fundamental to quality of life across the globe.
- It is vitally important that women are adequately represented in what has traditionally been, and is still, a male-dominated area.
- Science cannot reach its full potential unless it can benefit from the talents of the whole population, and until women and men can benefit equally from the opportunities it affords.

Further information on Athena Swan is at http://www.athenswan.org.uk/

TO APPLY

Apply online at: http://www.ucl.ac.uk/hr/jobs/   Search under Ref no: 1693683

Last update: 10/8/2017
You will need to register to use the system if you have not used it before and are able to do this after you have found the vacancy and clicked on the 'Apply now' button at the bottom of the online advert.

Thank you for your interest in this post and the Department of Chemistry at UCL