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| Job Description  |  |  | | --- | --- | | **Research Fellow in Computational Chemistry and Machine Learning** |  | | Department: ChemistryGrade: 7Location: UCL Bloomsbury Campus | 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 £37,332 to £39,980 per annum, including London Allowance of £5,000) with payment at Grade 7 being backdated to the date of final submission of the PhD thesis. | |  |

**LONDON’S GLOBAL UNIVERSITY**

**Department of Chemistry**

#### Reports to: Dr Tim Hele

#### Context

The post is funded through an Enhancement Award to Dr Hele’s Royal Society University Research Fellowship *Designer lighting: a radical approach to improve organic solar cells and light-emitting diodes*. This proposal aims to design molecular emitters for organic light-emitting diodes with emission throughout the visible and infra-red, to model the non-adiabatic dynamics of such systems and to design molecules for singlet fission downconversion. There are further aims of using Machine Learning and AI to accurately and reliably predict the spectra of organic radicals containing a variety of heteroatoms (chlorine, nitrogen, oxygen, sulphur etc), to extend the computational methodology to systems with multiple unpaired electrons such as diradicals, and to simulate the emission mechanism of organic light-emitting diodes.

The appointment is available to start immediately and in the first instance runs until 30th September 2025. Subject to funding and funder approval it may be extended to a duration of up to 28 months.

**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 3rd in the UK for 4\* submissions in REF 2021. 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 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>.

#### Main purpose of the job

The posthholder will be required to carry out research into:

* Simulation of possible intermediate electronic structures of emitter molecules to elucidate the radical emission mechanism
* Use Machine Learning and AI to improve algorithms for the simulation of radical electronic structure and excited states
* To extend electronic structure simulation algorithms to molecules with multiple unpaired electrons.

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**Duties and responsibilities:**

* To perform simulations of excited states of radicals, and their cation and anion forms.
* To use machine learning and AI develop improved algorithms for radical electronic structure simulation.
* To formulate algorithms to simulate the electronic structure of molecules with multiple unpaired electrons.
* To record, analyze and write up the results of calculations.
* To contribute to the drafting and submitting of papers to peer reviewed journals.
* To prepare progress reports on research for funding bodies as required.
* To contribute to the preparation and drafting of research bids and proposals.
* 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.
* To contribute to the induction and direction of other research staff and students as requested.
* 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

# Person specification

| **Criteria** | **Essential or Desirable** | **Assessment method**  **(Application/Interview)** |
| --- | --- | --- |
| **Qualifications, experience and knowledge** |  |  |
| PhD (or about to be awarded a PhD) in relevant subject area: Theoretical Chemistry or Physics | Essential | Application |
| Knowledge of Computer Programming | Essential | Application |
| Knowledge of quantum mechanics and experience in quantum chemistry calculations | Essential | Application, Interview |
| Experience of quantum chemical methods for excited state calculations | Essential | Application, Interview |
| Experience of working in a research environment | Essential | Application |
| Experience with Python Programming | Desirable | Application |
| GCSE English Grade C or above (or equivalent, e.g. IELTS) | Essential | Application |
| Experience of multi-disciplinary working | Desirable | Application |
| Experience with HPC | Essential | Application |
| Experience with radical electronic structure, machine learning and/or non-adiabatic dynamics | Desirable | Application, Interview |
| **Skills and abilities** |  |  |
| Proven research skills in quantum mechanics, especially electronic structure theory and/or non-adiabatic dynamics | Desirable | Application |
| Ability to analyse and write up data | Essential | Application |
| Ability to present complex information effectively to a range of audiences | Essential | Interview |
| Effective written and verbal communication skills in English | Essential | Application, Interview |
| **Personal attributes** |  |  |
| Commitment to high quality research | Essential | Interview |
| Ability to work collaboratively and as part of a team | Essential | Application/Interview |
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**General Information**

**Terms & Conditions of Employment**

The post is a UCL grade 7 post, the salary for which ranges from £42,099 to £50,585 per annum (including London Allowance of £5,000 p.a.). Starting salary is usually £42,099.

All posts that are based outside of London, for example at Harwell, will **not** have London Allowance included in the salary.

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 £37,332 to £39,980 per annum, including London Allowance of £5,000) with payment at Grade 7 being backdated to the date of final submission of the PhD thesis.

Some parts of the role can be undertaken remotely if necessary and the postholder will be required to work onsite at least one day a week.

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, teaching and professional services staff are at:

<https://www.ucl.ac.uk/human-resources/conditions-service-research-teaching-and-professional-services-staff>

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

**General information for Overseas Applicants**

<https://www.ucl.ac.uk/human-resources/working-ucl/employment-contract-administration-team/immigration>

<https://www.ucl.ac.uk/human-resources/working-ucl/relocating-uk-guide>

**Equal Opportunities**

[www.ucl.ac.uk/hr/docs/equal\_opportunity.pdf](http://www.ucl.ac.uk/hr/docs/equal_opportunity.pdf)

The Department has been awarded a Silver 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.athenaswan.org.uk/>

# Apply

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| To apply for this position visit:ucl.ac.uk/jobsSearch under Ref no:B04-04986 Please upload a CV, list of publications and cover letter outlining why you are interested in the role, and which of the essential and desirable criteria you meet and how, with your application.  Informal enquiries regarding the position can be directed to Dr Hele, [t.hele@ucl.ac.uk](mailto:t.hele@ucl.ac.uk). Informal enquiries related to the application process can be directed to [hr.chem@ucl.ac.uk](mailto:hr.chem@ucl.ac.uk).  . |