Job Description

Research Fellow in Biomedical Molecular Dynamics for Drug Discovery

Department: Chemistry

Grade: 7

Location: UCL Bloomsbury Campus

Reports to:

Professor Peter V. Coveney

Context

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.

Main purpose of the job

The successful candidate will join a very active inter-disciplinary group in the Centre for Computational Science, working on projects in fields ranging from condensed matter physics and chemistry to life sciences and medicine. A Ph.D. degree in biomolecular dynamics as used to perform free energy and related calculations of ligand-protein binding is essential, as is experience with high performance computing.

This post will involve the development of molecular models to support computer-based drug discovery and to investigate the biophysical and biochemical origins of drug resistance in pathologies such as HIV, cancer, and antimicrobial resistance, using established molecular dynamics codes such as NAMD and OpenMM. A key element of the approach is the development and use of automated workflows to assist in the rapid, accurate, precise and reproducible determination of binding affinities running on a range of ultra-high-end supercomputers, including Summit, number one in the Top500 list of supercomputers worldwide.

The post-holder will work closely with a large number of international projects across Europe and USA, and with collaborating industrial (pharma/biotech) and public sector partners who have an interest in exploiting our approaches in industry and healthcare.

Duties and responsibilities:

To carry out research under the supervision of the Director of the Centre for Computational Science (Professor P. V. Coveney), as follows:

- Development of patient specific molecular models and automated workflows in order to study and quantify the efficacy of ligand-protein binding through free energy and related calculations based primarily on NAMD and OpenMM molecular dynamics engibes; and to evaluate the performance of atomistic and coarse-grained molecular dynamics models, including on forthcoming exascale computers.
- Running of such models, simulations and workflows on workstations, clusters, supercomputers and on distributed e-infrastructure, nationally and internationally.
- The integration of such workflows into wider research e-infrastructures, so as to allow these modelling techniques to ultimately be used routinely in the pharmaceutical industry and clinical contexts.
- Preparation of research papers for publication in the scientific literature as well as regular reports and deliverables within various projects including CompBioMed (http://www.compbiomed.eu/); together with fully documented manuals describing the content of the software developed and used during the course of the appointment.

- Participation in regular meetings with colleagues at UCL and with colleagues in projects in which CCS is participating, including the reporting of results from the work being performed at UCL within these projects. This will entail some level of foreign travel. Participation in grant proposals and submissions.
- Assistance in the supervision of postgraduate and undergraduate students working on related computational projects within the CCS and more widely.
- The post-holder will carry out any other duties as are within the scope, spirit and purpose of the job as requested by Peter Coveney or the Head of Department.
- The post-holder will actively follow UCL policies including Equal Opportunities and Race Equality policies.
- The postholder will maintain an awareness and observation of Fire and Health & Safety Regulations.
- To undertake a limited amount of teaching in relation to subject area.
- 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 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
Qualifications, experience and knowledge	
PhD (or near to being awarded a PhD) in Biomolecular Dynamics modelling for protein-ligand binding free energy determination, with proven programming expertise in at least two languages (e.g. C++ and Python).	Essential
Experience with writing and executing automated workflows in distributed environments.	Essential
Experience in performing free energy calculations using both the ESMACS and TIES methods	Essential
Experience in running such free energy calculations in an automated manner on ultra-high end hardware on the path toward the emerging exascale	Essential
Experience in performing such free energy calculations on heterogenous architectures, in particular on computers with nodes comprising combinations of multiple cores and accelerators (primarily GPGPUs)	Essential
Have some experience of working with COVID-19 protein targets	Essential
Extensive experience of molecular modelling and simulation, particularly involving high performance (parallel) computing.	Essential
Experience of working with both NAMD and OpenMM molecular dynamics engines	Essential
High-quality publications at peer-reviewed journals: at least two published or accepted by the time of PhD award; for more experienced applicants, a correspondingly sustained output.	Essential
GCSE English Grade C or above (or equivalent, e.g. IELTS)	Essential
Experience with use of GPU architectures.	Essential
Skills and abilities	
Proven programming ability in at least two suitable high level programming language such as C, Fortran, Python and/or C++.	Essential
Excellent IT skills as required for performing post, including good knowledge of software and hardware infrastructure necessary for distributed environments.	Essential
Ability to develop and give advice on strategic decisions within this domain.	Essential
Personal attributes	
Good presentational skills.	Desirable
Excellent interpersonal relations with junior and senior staff, and excellent networking skills.	Desirable
Ability to work alone as well as within a group.	Essential

Criteria	Essential or Desirable
Self-motivated and able to use his/her initiative.	Desirable
Willingness to travel for European and other international meetings.	Desirable
Effective organisational skills.	Essential
Practical problem solving under time constraints and the ability to work to deadlines.	Desirable
Clear, comprehensive and technically correct communication (English - written and oral), as the post holder will be required to write reports, papers, presentations and documentation.	Essential
The ability to learn quickly and assimilate large amounts of information, and present this confidently in meetings.	Desirable

General Information

Terms & Conditions of Employment
The post is initially funded for 24 months at grade 7, the salary for which ranges from £35,965 to £43,470 per annum (including London Allowance of £3,148 p.a.). Starting salary is usually £35,965.

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 £31,479 to £33,194 per annum, including London Allowance of £3,148 p.a.) 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, 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

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.athenaswan.org.uk/

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