The Project
The successful candidate will join a very active inter-disciplinary group in the Centre for Computational Science, and will work on the development of state of the art classical molecular dynamics codes for use in advanced materials and personalised medicine research. These codes will run on high performance supercomputers. A Ph.D. degree—involving a substantial high-performance computing component—in Chemistry, Physics, Applied Mathematics or Computational Biology, with experience of molecular dynamics simulation, is a minimal requirement. Experience in parallel programming for high performance computing environments is essential, including for accelerators (such as GPU and FPGA), alongside a proven ability to write code for applications in at least one of these two application domains.

Main Purpose
The postholder will develop and optimise verified and validated molecular dynamics simulation for advanced materials and drug discovery based on or around established molecular dynamics codes such as OpenMM, LAMMPS, NAMD and GROMACS and drawing on modern techniques for uncertainty quantification. The codes will be optimised for existing and future emerging architectures along the path to the exascale. The postholder will also be involved in building and applying complex workflows which can be deployed within high performance computing environments, including clouds; and he/she will provide support for the computing systems at the Centre for Computational Science. The ultimate aims of this research are to advance our capacity to perform large scale, high throughput, certifiable, multiscale materials and ligand-protein/nucleic acid modelling research.

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 extremely fast classical molecular dynamics codes, based on or around established molecular dynamics codes such as LAMMPS, OpenMM, NAMD and GROMACS, for research in advanced materials and personalised medicine.

- Running of such models on workstations, clusters, clouds and supercomputers nationally and internationally, including on machines enhanced with accelerators including GPUs and FPGAs.
• Enhancing and developing existing tools to automate the running of molecular dynamics calculations in stand-alone mode for as well as within the context of integrated multiscale modelling environments.

• The integration of models into the wider research infrastructure, to allow such modelling techniques to be enjoy routine use by end-users.

• Preparation of research papers for publication in the scientific literature; and of fully documented manuals describing the content of the codes used and developed 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 and assistance in the reporting of results from the work being performed at UCL within these projects. This will entail some level of foreign travel, particularly to Europe for purposes of collaboration with ongoing European-funded projects. Participation in preparation and submission of future grant applications.

• Assistance in the supervision of post-graduate and undergraduate students working on related computational projects within the CCS and more widely.

• The postholder is required to undertake a limited amount of teaching in relation to the subject area.

• The postholder 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 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 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

Knowledge – including Qualifications
A PhD degree in Chemistry, Physics, Applied Mathematics, Computational Biology or related areas, with a significant component of bio-molecular modelling and simulation and proven programming expertise. (Essential)
GCSE English Grade C or above (or equivalent, e.g. IELTS) (Essential)

Experience
Extensive experience of biological molecular modelling and simulation, involving high performance computing. (Essential)
Experience using common molecular dynamics packages such as NAMD, OpenMM, GROMACS and LAMMPS. (Essential)
Experience of coding for and using GPU and/or FPGA accelerated molecular dynamics codes. (Essential)
Proven parallel programming ability in one high level language (such as Fortran, C, C++) and one scripting language (e.g. Python). (Essential)
Excellent IT skills as required for performing post, including good knowledge of software and hardware tools used in HPC environments, at the terascale and above. (Essential)
Ability to develop and give advice on strategic decisions in this domain. (Desirable)

Skills & Abilities
A proven ability to programme quickly and effectively in state-of-the-art high-performance computing environments including those with accelerators. (Essential)
An ability to work alone as well as within a group. (Essential)
Excellent organisational skills. (Essential)
Clear, comprehensive and technically correct communication (English - written and oral), as the postholder will be required to write reports, papers, presentations and documentation. (Essential)
Excellent interpersonal relations with junior and senior staff, and excellent networking skills. (Essential)
Good presentational skills. (Desirable)
The ability to learn quickly and assimilate large amounts of information, and present this confidently in meetings. (Desirable)
Practical problem solving under time constraints and the ability to work to deadlines. (Desirable)

Personal Qualities
Must demonstrate a consistently high standard in achievements and impact throughout career to date. (Essential)
Willingness to travel for European and other international meetings. (Essential)
Self-motivated and able to use their initiative. (Desirable)

Other
An excellent and consistent publication track record including at least two high quality scientific publications for newly graduated PhD applicants (these may be in press) and proportionately more with increasing post-doctoral experience (Essential)

General Information

Terms & Conditions of Employment
The appointment is for 18 months in the first instance, starting on 1st February 2018 or soon thereafter. 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 is usually £34,635. Progression through the salary scale is incremental.

Last updated 16/3/2015
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 6 (salary £30,316 to £31,967 p.a. (inclusive of London Allowance) with payment at Grade 7 being backdated to the date of final submission (including corrections) of the PhD thesis. 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
UCL recognises that in our society, individuals and groups are discriminated against both directly and indirectly on the grounds of: age, colour, disability, ethnic origin, gender, HIV status, marital, social or economic status, nationality, race, religious beliefs, responsibility for dependants, sexual orientation, trades union membership or unrelated criminal convictions.

To counteract discrimination, UCL is committed to actively opposing all forms of discrimination, raising awareness and tackling the causes and consequences. It is committed to providing a learning and working environment in which the rights and dignity of all its members are respected and which is free from discrimination, prejudice, intimidation and all forms of harassment including bullying; to making staff and students feel valued, motivated and enabled to do their best work and to creating a safe, welcoming working environment accessible to all.

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/

TO APPLY

Apply online at: http://www.ucl.ac.uk/hr/jobs/ under Ref no: 1700766

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 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