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| Job Description |  |
| Computational Support Officer  | Grade: 7, Full-time, 36.5 hours |
| Department: Chemistry | Location: Bloomsbury Campus |

#### Reports to

**LONDON’S GLOBAL UNIVERSITY**

**UCL PROFESSIONAL SERVICES ROLES**

Professor Graham Worth with professional accountability to the Departmental Manager.

#### Context

**Faculty of Mathematical & Physical Sciences:**

The Faculty of Mathematical & Physical Sciences comprises: Chemistry Department, Earth Sciences Department, Mathematics Department, London Centre For Nanotechnology, Physics & Astronomy Department, Science & Technology Studies Department, Space & Climate Physics & Mullard Space Science Laboratory, Statistical Science Department, Institute for Materials Discovery and Institute for Risk & Disaster Reduction.

**The Chemistry Department:**

The Chemistry Department at UCL is the oldest in England, and today is one of the best in the UK, in REF 2021 it was ranked joint 1st nationally for 4/3\* research. 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 is committed to supporting excellence in both research and teaching and offers undergraduate BSc and MSci programmes in Chemistry and currently teaches over 600 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 80 students per year and has an overall Postgraduate Research student school of about 250 students.

The Chemistry Department has over 55 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. Details about our research can be found at <http://www.ucl.ac.uk/chemistry>.

#### Main purpose of the job

The postholder is one of three departmental Computational support staff. They will work as part of this team to provide support to staff and students across a range of platforms. This role will manage and develop the computational chemistry clusters currently including eight multi-processor linux clusters and support specialized computational chemistry research in the department.

#### Duties and responsibilities

1. **Managing, maintaining and developing the computational chemistry facilities of the chemistry department, comprising a number of multiprocessor linux/unix clusters (ranging in architecture and uses), fileservers and associated hardware including:**
* Replacing failed CPUs, disks and other components.
* Ensuring secure and efficient operation, implementing queuing/resource management systems, checking regularly for security breaches and anomalous activity, monitoring air-conditioning and power supply.
* Carrying out appropriate maintenance and upgrades, including daily security patches.
* Installation of specialist software packages, license management of software on both
Departmental and University facilities.
* Addressing requirements for managing data and for connection of local resources to those elsewhere in UCL, UK, EU and overseas.
* Data backup/archiving, implementing and disaster recovery.
* User support, assisting individual users in accessing facilities, providing up to date information to the user base.
* Support of clusters run by the Chemistry Department and stored outside the Department.
1. **Advising on the implementation of applications on appropriate platforms and responsible for demonstrating and training students and staff in the use of computational tools to enable their learning and research including:**
* Training undergraduates on the use of required software on-line and in workshops.
* Training in the use of linux for research-led computational chemistry laboratory work for both undergraduate and postgraduate teaching.
* Training in core skills in linux and computational packages used by research students and staff.
1. **Managing the procurement and installation of new systems and rationalisation of current systems as appropriate, including:**
* Adding and replacing new hardware to update and extend existing clusters.
* Planning and managing an effective local data storage solution with adequate external connectivity for large-scale data transfers.
* Acting as an advocate for computation chemistry with the UCL Research Computing environment to ensure that the most effective use is made of the supercomputing facilities (e.g. Myriad and Kathleen), training and support available centrally.
* Providing technical advice to academic staff developing the computational chemistry strategy of the department.
1. **Departmental Computer Representative**
* To act as a liaison between the department and central ISD, providing feedback to central services, whilst also ensuring appropriate implementation of central policies within the department.
* Work with central services to provide solutions for problems impacting the department including those related to centralized computing, managed equipment, or infrastructure requirements. This may involve directing users to correct ISD procedures or contact.
* Participate in relevant networks and meetings to keep abreast of UCL developments and ensure these form part of work undertaken by the computer support team.
1. **Miscellaneous**
* Work with other computing support staff within the department to ensure full cover across all areas of IT support during peak periods.
* Maintaining high standards of record keeping, whilst ensuring adherence to confidentiality and GDPR requirements.
* The post holder will contribute to departmental, faculty and UCL-wide working groups, committees or communities of practice as requested.
* The post holder will maintain own continuing professional development.

This 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 post holder will actively follow UCL policies including Equal Opportunities policies 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 post holder will maintain an awareness and observation of Fire and Health & Safety Regulations.

# Person Specification

| **Criteria** | **Essential or Desirable** | **Assessment method****(Application/Interview)** |
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| **Qualifications, experience and knowledge** |  |  |
| A good first degree involving computation chemistry or a closely-related discipline | Essential | Application |
| A PhD or equivalent experience of research in computational chemistry, or a closely-related discipline. | Essential | Application |
| Thorough knowledge of unix/linux as a cluster administrator and programmer | Essential | Application/Interview |
| Knowledge of some scientific programme languages (e.g. FORTRAN, C, Java) | Essential | Application/Interview |
| Knowledge of Computer networking | Essential | Application/Interview |
| GCSE English Grace C or above (or equivalent, e.g. IELTS) | Essential | Application/Interview |
| Knowledge of Windows and Mac operating systems | Desirable |  Application/Interview |
| Knowledge of the legal position around computer use and data storage | Desirable |  Application/Interview |
| **Skills and abilities** |  |  |
| Ability to set-up, install and maintain computers | Essential | Application/Interview |
| Experience and evidence of competency in the set-up and management of unix/linux systems | Essential | Application/Interview |
| Ability to communicate effectively in technical discussions with staff and students with differing levels of understanding from novices to experts | Essential | Application/Interview |
| An interest in and the ability to keep up to date with current computing, networking and scientific computing techniques | Essential | Application/Interview |
| Ability to support specialist applications in quantum chemistry, atomistic and multiscale molecular modelling | Desirable | Application/Interview |
| Experience of supporting a large group, in the order of 100 registered users and networked computers | Desirable | Application/Interview |
| Experience/Knowledge of parallel computing, including installation of parallel codes | Desirable | Application/Interview |
| Experience with compiling parallel code (MPI, OpenMP) and linking of code to external libraries (MKL, BLAS, LAPACK) | Desirable | Application/Interview |
| Experience of computer hardware procurement | Desirable | Application/Interview |
| [**UCL Ways of Working**](https://www.ucl.ac.uk/human-resources/policies-advice/ways-working) |  |  |
| Promoting personal and professional development. | Essential | Interview |
| Anticipating issues and adjusting approaches when necessary | Essential | Interview |

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