

# UNIVERSITY COLLEGE LONDON

## Job Description

<b>Job Title:</b>	Research Associate in Computational Modelling of the Organic Solid State
<b>Department:</b>	Chemistry
<b>Reports to</b>	Prof Sarah (Sally) L Price PI on project.
<b>Grade:</b>	Grade 7

### Main Purpose

The postholder will be required to carry out computational research in the area of computational organic crystal structure prediction and surface science, as defined in the proposal “Computationally Designed Templates for Exquisite Control of Polymorphic Form” EP/K039229/1. This requires working collaboratively with the experimental researchers to complete this major 4 year project, computing crystal energy landscapes and surface modelling for organic systems, including the development and testing of programs, recording, analysing and writing up the results as part of a research team.

### Duties and Responsibilities

- To continue development of the computational methods of searching for energetically feasible crystal structures for an organic molecule by increasing the accuracy of the relative energies to make confident predictions that unknown polymorphs are thermodynamically feasible. To contribute to the adaptation of tools developed during the Basic Technology project “Control and Prediction of the Organic Solid State” (CPOSS [www.cposs.org.uk](http://www.cposs.org.uk) ). To develop the use of computer codes for modelling organic molecules interacting with crystal surfaces, including defects. To use both anisotropic atom-atom model potentials and electronic structure (molecular and periodic) approaches as appropriate.
- To run computational experiments, as part of collaborations with other CPOSS groups, ensuring that experiments are appropriately supervised and supported. To record, analyse and write up the results of experiments.
- To contribute to the training of new research staff, students and outside groups, including industrial scientists, in the use of the computational tools.
- To maintain the computational infrastructure in support of the work of other members of the group. To maintain the computer system of doing polymorph searches and depositing the results in the database.
- To prepare and present findings of research activity to colleagues for review purposes.

- To contribute to the drafting and submitting of papers to appropriate 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.
- As duties and responsibilities change, the job description will be reviewed and amended in consultation with the postholder
- 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 (Prof S.L. Price) or Head of Department/Division
- The postholder 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.

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## Department of Chemistry

### Person Specification for the Post of Research Associate in Computational Modelling of the Organic Solid State

#### Knowledge – including Qualifications

A PhD involving creative use of computational chemistry techniques is essential.

Knowledge of a range of computational chemistry methods is essential, preferably including both electronic structure and atomistic crystal modelling codes. Ability to adapt existing computer codes and experience with DMACRYS and other codes using distributed multipoles e.g. ORIENT is desirable.

An ability to create efficient workflows for analysing and moving data between computer applications is essential.

Basic knowledge of the mathematical description of organic crystal structures is highly desirable.

An ability to work in collaboration with scientists with both an experimental and computational background is essential.

#### Skills

Essential:

Basic research skills in computational chemistry

Programming and scripting experience in Unix environments

Ability to handle large sets of computer files

Ability to analyse and write up data

Ability to present complex information effectively to a range of audiences

Effective written and verbal communication skills

#### Experience

Essential:

Experience of working in a research environment

Desirable:

Experience of multi-disciplinary working, particularly working with experimentalists.

#### Personal Qualities

Essential:

Commitment to high quality research over a sustained 4 year project.

Ability to work collaboratively and as part of a team.

Commitment to UCL's policy of equal opportunity and the ability to work harmoniously with colleagues and students of all cultures and backgrounds