





# UCL Industrial Doctorate Centre in Molecular Modelling & Materials Science

The Industrial Doctorate Centre in Molecular Modelling and Materials Science at University College London (M<sup>3</sup>S IDC), UK trains and supports researchers in all areas of computational and experimental materials science. The M<sup>3</sup>S programme is highly interdisciplinary, with students based in a growing number of UCL science, engineering and biomedical departments. The background of the students is similarly varied, ranging from degrees in the chemical and medicinal sciences to physics, computer science and engineering. Most of the Centre's students are recent graduates but others already have significant work experience in industry, but find that doctoral research will broaden their experience and enhance their career prospects.

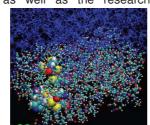
Established in 2005 as a virtual Centre, extensive investment by UCL over the years has provided the M<sup>3</sup>S IDC with modern training facilities and dedicated research labs to support 10-15 new graduate researchers each year. The four-year programme is targeted at future research leaders in industry, or scientists and engineers who wish to maintain significant links with industry in an academic career. The training covers a broad range of topics, from technical courses on computer modelling techniques and the materials sciences to business development and project management. Professional development. knowledge transfer and responsible innovation are also included to provide the students with a comprehensive set of generic and transferable skills.

Research in the Centre focuses on four topical areas:

#### **Catalysis and Energy Materials**

One of the founding research areas in the M<sup>3</sup>S IDC, catalysis remains a topical field owing both to its sustained sponsorship by a number of companies, including Johnson Matthey and Exxon Mobil, as well as the research

expertise in this area within UCL. Present research includes the heterogeneous catalysis of redox processes on transition-metal oxides and supported metal clusters, as well as the design of novel nano-catalysts and microporous composite



materials for  $CO_2$  conversion and production of chemical feedstock compounds. Energy Materials is a related, but relatively newer area of research, sparked by the growing interest by oil companies and energy providers, as well as a recent confluence within UCL of new and existing expertise in the areas of solid fuel cells, novel materials for hydrogen storage and clean/renewable energy, in addition to ongoing research into energy waste, such as radiation damage containment and  $CO_2$  sequestration.

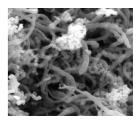
#### Nano-engineering for Smart Materials

Design at the nano-level of smart materials, which respond rapidly and often reversibly to changes in their immediate environment, is a highly topical area of research. One application in the M3S IDC is in the response of glass to heat and light, where M<sup>3</sup>S investigators have teamed up with Pilkington to design self-cleaning and self-cooling window glasses. Other triggers for smart materials include tailored solubility, for example in glasses for slow drug release and magnetism, all of which areas are represented strongly in UCL and have important industrial applications, for example in building design and healthcare applications.

## Materials for Bio-Medical Applications and Pharmaceuticals

Bio-materials science is a rapidly expanding field of research within the Centre, with research efforts ranging

from the custom-design of massive bone implants, to the development of tailored bio-glasses, magnetic contrast agents and tissue characterization and engineering. Also within the healthcare remit is one of the key problems facing the pharmaceutical industry,



namely the large number of possible polymorphs that can exist for any one drug, which may compromise its effectiveness and ultimately can have repercussions for patients and patents. UCL researchers have shown pharma companies that computational structure prediction and experimental testing can successfully screen potential drug polymorphs, before costly manufacturing and in vivo testing need ever take place.

### Information Technology and Software Engineering

Multi-scale modelling, e-science and grid technology is developed within the Centre in collaboration with a number of international developers of computer software, e.g. Accelrys, whereas the design and engineering of materials for the electronics industry has been added more recently to the M3S portfolio, with current research focused on the development of high gate semiconductor devices and highly accurate and sensitive signal detection equipment.

Core-funded by the UK Engineering and Physical Sciences Research Council, external collaborators are invited to part-sponsor individual students to work on topics directly relevant to their own research and development programmes. The external sponsors are involved with the research project from the outset and often provide placements for the student in their own research laboratories. External collaborators of the M<sup>3</sup>S IDC students vary from large multi-national corporations to medium-sized or start-up companies and national research laboratories.







# **Programme Structure**

The integrated 4-year doctoral training programme in the M<sup>3</sup>S ICDT combines a one-year Master of Research (Mres) programme with a subsequent three-year doctoral research programme.

## **MRes programme**

The MRes programme incorporates a number of different training and research activities:

- Dedicated taught courses in molecular modelling, materials science and topic-specific courses.
- Survey and review of the relevant scientific literature.
- Research project, which comprises 60% of the MRes degree programme.
- Intensive Project Management training, which is accredited by the Association of Project Managers, who confer Associate Membership on the student upon successful completion of the course.
- Professional, generic and transferable skills training provided by the UCL Centre for the Advancement of Learning and Teaching.
- Optional elective courses at the London Business School.

Upon successful completion of the first year, the degree of MRes is conferred and the students proceed to the second phase.

## **Doctoral Research Programme**

The second phase consists of a three-year doctoral research programme, where each student works in

collaboration with an external sponsor. The student may be placed with the external sponsor for short or long periods and is sometimes fully integrated in the Research team of the sponsor. The EngD degree is conferred upon successful completion of novel and high quality research, submission of a written doctoral thesis and viva voce examination by external examiner.

## **Application Procedure**

Applications are invited all year round for entry into the M<sup>3</sup>S programme. Final year undergraduate or master students with background in Chemistry, physics and materials science are particularly welcomed to apply.

If you are interested in the M<sup>3</sup>S programme, please email your CV, transcript which covers the courses you have taken during your undergraduate and postgraduate (if any) study and a one-page statement explaining why you wish to follow this programme to Dr Zhimei Du: <u>z.du@ucl.ac.uk</u> ( both English or Chinese are fine)

Your CV should include details of your academic qualifications and the contact details of two referees, one of whom should be familiar with your research career to date.

For successful candidates, UCL will provide full tuition fees and will assist the candidates to apply the CSC (the China scholarships Council), Scholarship, which will cover the living expense of the candidate during their study in UK.

