UCL Industrial Doctorate Centre in Molecular Modelling & Materials Science

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UCL

Doctoral Research in Partnership with Industry

EPSRC

Introduction

History and Vision

Established in 2005, the ***M³S IDC*** is funded by ***EPSRC*** and co-sponsored by ***industrial partners***.

Our vision is to develop a fundamental understanding of the effect of molecular-level processes on macroscopic materials properties and hence to improve the design and engineering of functional materials for applications in energy, nanoscience, catalysis, information technology and biomedical science and engineering.

Multi-disciplinarity

The ***M³S IDC*** bridges the UCL Faculties of Mathematical & Physical Sciences, Biomedical sciences and Engineering, with students registered in, for example, UCL departments of Chemistry, Chemical Engineering, Physics, Earth Sciences, Electrical & Electronic Engineering, Civil Engineering and the London Centre for Nanotechnology, Eastman Dental Institute and the Institute of Orthopaedics.

Industrial Partners

The ***M³S IDC*** sponsoring companies span an wide range of industrial interests both in UK and abroad. So far, **27** industrial collaborators sponsor studentships.

In terms of the size, both small and medium enterprises and multi-national corporations have been involved in the research activities of the ***M³S IDC***, including:

- **Energy providers and catalyst specialists**
  e.g. Exxon Mobil, Johnson Matthey
- **Glass manufacturers**
  e.g. Pilkington Glass UK, Asahi Glass Japan
- **Computing hardware and software companies**
  e.g. Silicon Graphics, Accelrys Ltd
- **Biomedical Applications**
  e.g. Stanmore Implants Worldwide, Straumann AG
- **National laboratories**
  e.g. Diamond, ISIS, the Met Office, ESRF, NPL, UK
  US Pacific Northwest National Laboratories

Pilkington · TWI · AGCC · ExxonMobil · Met Office Consulting · Johnson Matthey · sgt · accelrys

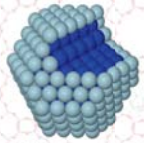
For further information on joining the M3S IDC as a student or external collaborator, please contact Professor Nora de Leeuw on n.h.deleeuw@ucl.ac.uk

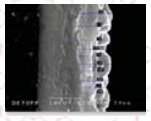
Research Themes

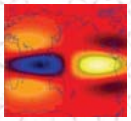
The ***M³S IDC*** runs a significant **internationally** leading research programme in the areas of computer modelling and materials science to develop fundamental understanding of the effect of molecular-level processes on macroscopic materials properties and hence to improve the design and engineering of functional materials.

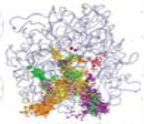
Main research themes

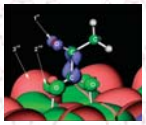
- Energy materials and catalysis.
- Clean and renewable energy.
- Carbon capture and storage.
- Smart materials
- Nano-science and nano-engineering.
- Pharmaceuticals and bio-medical engineering.











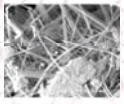
Examples of Research Projects Carried out by Our Students

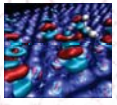
Christopher Downing is sponsored by **the Science Technology Facilities Council**, **UK** to apply computational techniques to investigate a catalyst which can enable the transformation of CO_2 to an environmentally benign, or a useful energy storage medium such as methanol or dimethyl ether.

Sacha Noimark works on a project (sponsored by **Ondine Bipharma)** to develop a novel approach against catheter-related infections.

Liam Bennett and Tom Daley are both sponsored by **Johnson Matthey Catalysts. Liam** gets engaged in a computational study of oxidative and reductive properties of CeO_2 while Tom has used *ex situ* and *in situ* methods to determine atomic-architecture of model catalytic materials

Kay Rigby, Isaac Sugden and Elisabeth Krizek are working on projects focused on the behaviour of nuclear materials. The projects are sponsored by **AWE.**.





Doctoral Training Programme

We provide students with training not only in cutting-edge research technologies, but also in the development of business and entrepreneurial as well as transferable skills - key elements that are highly sought-after by employers in industry, academia and business.

The training programme in the ***M³S IDC*** is structured as a 1+3 course, with a taught first year, leading to an ***MRes*** in Molecular Modelling and Materials Science, followed by a three-year doctoral research degree.

Key features of the ***M³S IDC*** training programme

- Technical lectures given by academic and industrial scientists
- Accredited Project Management and Business courses
  e.g. APMP and London Business School courses
- Materials simulation group project
- Transferable skills training, including:

IT skills, archive and library resourcing, languages, thesis preparation, presentation skills, entrepreneurship & innovation management and teaching skills

- Engagement with stakeholders

Annual Industry Convention

- Hold once a year at the end of June in UCL.
- Participants: Industrial sponsors, UCL academic staff and students of M³S IDC.
- Activities: ***A keynote talk by a prominent industrial scientist;***
  Networking and interacting among the participants;
  Generating new collaborations and research ideas;
  Oral presentations given by first year EngD students;
  Poster displacement.

Sixth Form Event

- **Aim:** Provide students with valuable experiences of pooling expertise and resources to organise a major project to a deadline.
- **Who:** Second year EngD students
- **What**: Organise a sixth form event for London-wide schools with a given budget and to take in charge of all aspects of the vents, including:
  promotion, registration, programme design and printing, exhibitions, catering, sponsorship, entertainment, etc