Theory of Condensed Matter

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Quantum Mechanical Modelling of Biological Function

Our understanding of many atomic scale processes in the physical sciences has been transformed by quantum mechanical simulations. We are developing on a range of new simulation technologies that will extend this capability to new phenomena and to new areas of scientific investigation. Quantum mechanical calculations on systems containing many thousands of atoms and techniques are now emerging that will allow us to sample the complex configuration spaces of biological molecules. Together, these methodologies will bring us to the beginning of the era of quantum mechanical simulation of biological function.

Recent calculations on the binding of oxygen and carbon monoxide to heme, the kernel of the haemoglobin metalloprotein central to human respiration, indicate the binding depends on a number of subtle quantum mechanical effects, including quantum entanglement.

Alex Chin and Mike Payne

Mechanics of Soft Solids

Liquid crystal elastomers are soft solids that combine the orientational order of liquid crystals with the large deformation mechanics of rubbers, resulting in huge reversible shape changes when the LC order is destroyed by heat or illumination. Conversely, the LC order can be manipulated by imposing shape changes, leading cholesteric elastomers to change from red to blue on stretching. An exciting new area is blue phase LC elastomers which contain true periodic crystal order with optical lattice spacing, making them stretchy photonic crystals.

Mark Warner

The Composition Catwalk: Designer Materials

Through the stone, bronze, and iron ages the discovery of materials has chronicled human history. The coming of each age was sparked by a chance discovery of a new material. Despite the central importance of materials in enabling new technologies, even today the leading approach to develop new materials is experiment driven trial and error. We have developed a new computational tool that can automatically design a material with specified physical properties, and have proven its accuracy by predicting several new alloy families that were subsequently experimentally verified. Each alloy has eight individual physical properties that match or exceed commercially available materials so they are now undergoing compliance testing and further development by Rolls-Royce plc.

With the materials design approach proven on metal alloys, future projects will involve working with industrial partners Rolls-Royce plc and Samsung Electronics to exploit first principles computational techniques to extend the materials design approach to other alloy systems, semiconductors, and beyond.

Gareth Conduit

Effects of Irradiation in Matter

A lot of interesting physics happens when irradiating matter with high-energy particles. Its study is of great relevance in contexts as important as the radiation therapy of cancer (shooting H or C ions onto living tissue), the effect of cosmic rays in materials and devices in space or airplanes (mostly high-energy protons and alpha particles), or the durability of materials for the nuclear industry (new fusion technology, or dealing with existing nuclear waste).

The relevant processes are not adiabatic in many cases, meaning that we cannot rely on simulations that matter assuming the equilibrium behaviour of the electrons in matter, but rather we need to follow these dynamics finding time-evolving solutions for the quantum dynamics in the problem, which is done using time-dependent density-functional theory.

Emilio Artacho

Random Numbers for Quantum Correlation and Predicting Structures

Although it may seem surprising at first, random numbers can be used to help solve complicated problems in physics. In Monte Carlo methods repeated random sampling is used to compute results of many random processes of freedom. In quantum mechanics, the state of a system of N particles is described by a many-body wavefunction, which is a 2N-dimensional function using a standard mathematical technique. Quantum Monte Carlo offers an alternative and efficient approach which accurately describes the interactions between particles. Electrons repel one another, because according to quantum mechanics they must obey the Pauli exclusion principle. This results in a `hole' being created around each electron, from which other electrons are excluded. The figure on the right shows the hole created by an electron in a real solid as calculated by Quantum Monte Carlo.

What structure will be formed if four parts hydrogen and one part silicon are mixed?

At low pressures they phase separate but at high pressures they form the highly symmetrical insulating crystal shown on the left. This result was obtained using `density-functional theory' methods based on random numbers, and it was subsequently confirmed by experiment. These techniques can be used to explore structures and `discover' new materials.

Richard Needs

Materials Discovery

The creation of new materials is difficult and expensive. It is difficult to “see” the structure of these materials over the length scales that they work, and expensive to create prototype materials. Whilst experimental physics can use x-rays, high energy electrons or lasers to infer the structure of these materials, this process is made much more robust by containing double helices when combined with theoretical predictions of the kinds of structures that can be formed. We use quantum mechanics algorithms based on the results of these experiments, helping to understand and suggest new high-performance materials. The theoretical prediction of even very simple structures has, until recently, been out of bounds due to the large number of possible atomic arrangements. The ab initio random structure searching method (AIRSS) uses a stochastic approach to suggest different structural configurations of atoms within a material.

There is substantial interest in enhancing the capacity of lithium ion batteries (LIBs), driven by the economic and environmental advantages of increasing the range of electric vehicles, and enabling longer life portable electronic devices. The traditional anode is composed of graphite but recently silicon has been suggested as an alternative which has a theoretical capacity some ten times larger. Silicon anodes are not fully understood and suffer from large volume expansion on charge and hysteresis on charge cycling. By searching over a range of stoichiometries we can model how a battery is charged, predicting the structural changes of the electrodes as a charging potential is applied. From this initial step we perform further theoretical analysis such as NMR and EELS (electron energy loss) spectroscopies and predict charge and discharge voltages.

Many important technologically relevant materials cannot be reached within a single crystalline structure. We develop models to also encompass the shortand longrange disorder in materials in order to accurately predict their properties. For example, point defects can drastically change both the electronic properties of semiconductors and the physical properties of high-performance alloys. Beyond point defects, both site disorder and short-range play a role in lithium battery electrodes.

Andrew Morris

EPSRC Centre for Doctoral Training in Computational Methods for Materials Science

October 2016 will see the third cohort of students join the Centre for Doctoral Training in Computational Methods for Materials Science. This CDT provides a fully-funded four-year PhD programme incorporating the taught element of the existing MPhil in Scientific Computing in the final year. EPSRC-funded places are available for eligible candidates, as are numerous externally-funded projects in collaboration with industrial partners.

The development of new materials lies at the heart of many of the technological challenges we currently face, for example creating advanced materials for energy generation. Computational modelling plays an increasingly important role in the understanding, development and optimisation of new materials.

Our CDT will train young scientists not only in the use of existing modelling methods but also in the underlying computational and mathematical techniques. This will allow them to develop and enhance existing methods, for instance by introducing new capabilities and functionalities, and also to create innovative new software tools for materials modelling in industrial and academic research.

Professor Mike Payne

Contacts

For general details about postgraduate admissions, see http://www.tcm.phy.cam.ac.uk/vacancies/postgrad.html. To contact a particular staff member, please use the contact details below.

Dr Sebastian Ahrent
Prof. Emilio Artacho
Dr Claudio Castelnovo
Alex Chin
Dr Gareth Conduit
Prof. Nigel Cooper
Dr Dmitry Kovrizhin
Dr Aston Lamarcq
Dr Gunnar Möller
Dr Andrew Morris
Prof. Richard Needs
Dr Andreas Nuenenkamp
Prof. Mike Payne
Prof. Ben Simons
Prof. Mark Warner
sea31@cam.ac.uk
ea245@cam.ac.uk
c7260@cam.ac.uk
ac307@cam.ac.uk
ghj29@cam.ac.uk
rm25@cam.ac.uk
dk87@cam.ac.uk
aj2010@cam.ac.uk
fum386@cam.ac.uk
ajm255@cam.ac.uk
m11@cam.ac.uk
Evan44@cam.ac.uk
mcp1@cam.ac.uk
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http://www.tcm.phy.cam.ac.uk/profiles/fum386/
http://www.tcm.phy.cam.ac.uk/profiles/ajm255/
http://www.tcm.phy.cam.ac.uk/profiles/m11/
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