Theory of Condensed Matter

TCM and CDT graduate admission web pages

http://www.tcm.phy.cam.ac.uk/vacancies/postgrad.html

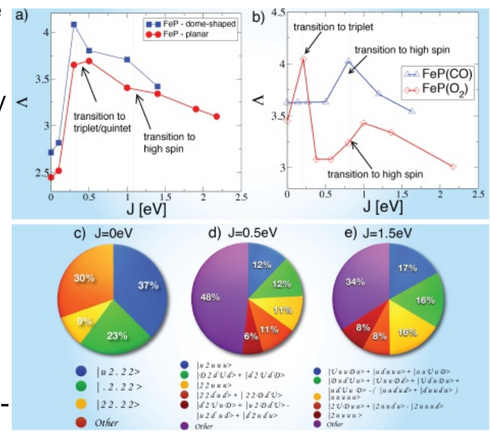
https://www.csc.cam.ac.uk/academic/cdtcompmat

Quantum mechanical modelling of biological function

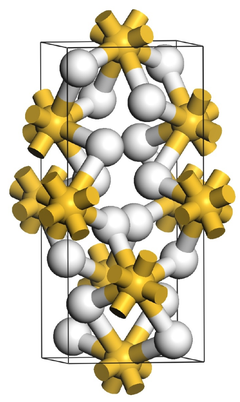
Our understanding of many atomic scale processes in the physical sciences has been transformed by quantum mechanical simulations. We are developing a range of new simulation technologies that will extend this capability to biological problems. We can already perform quantum mechanical calculations on 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 prediction of biological function.

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

Mike Payne



(a) and (b) Von Neumann entanglement as a function of the Hund's coupling on the iron atom, J, for various heme systems. (c-e) occupancy of iron orbitals for dome shaped heme for three values of J. Note that the actual value of J for an iron atom is roughly 0.8eV.



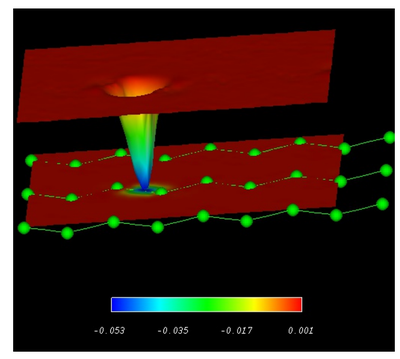
Random numbers for quantum correlation and predicting structures

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 for systems which have many degrees of freedom. In quantum mechanics, the state of a system of *N* particles is described by a many-body wave-function which is a 3*N*-dimensional quantity and is impossible to calculate exactly 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 they are charged and because 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.

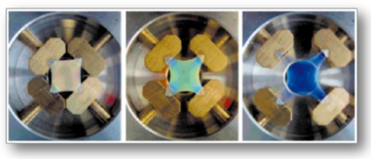
What structure will be formed if four parts hydrogen and one part silicon are mixed? At low pressures they phase separate but at high pressures they form the highly symmetrical insulating crystal shown on the left. This result was obtained using 'density functional theory' methods and a searching algorithm 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



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.

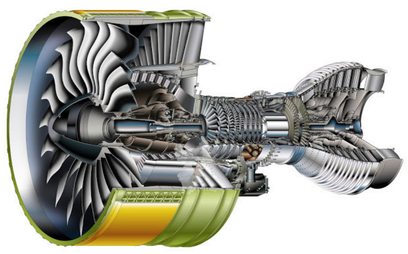


Colour changes when a cholesteric elastomer is stretched.

Mark Warner

The Composition Catwalk: Designer Materials

Through the stone, bronze, and iron ages the discovery of new 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 alternatives so they are now undergoing compliance testing and further development by Rolls Royce plc.

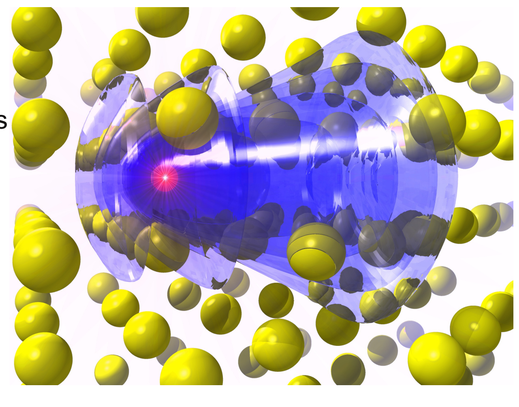


With the materials design approach proven on metal alloys, future projects will involve working with industrial partners Rolls Royce plc and Samsung Electronics to exploit first principles computational techniques to extend the materials design approach to other alloy systems, semiconductors, and beyond.

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 ion radiotherapy 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 of matter assuming the equilibrium behaviour of the electrons in matter, but rather we need to follow their dynamics finding time evolving solutions for the quantum dynamics in the problem, which is done using time dependent density functional theory.



Emilio Artacho

EPSRC Centre for Doctoral Training in Computational Methods for Materials Science

October 2018 will see the fifth cohort of students join the Centre for Doctoral Training in Computational Methods for Materials Science. This CDT provides a fully funded four year PhD course incorporating the taught element of the existing MPhil in Scientific Computing in the first year. EPRSC 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

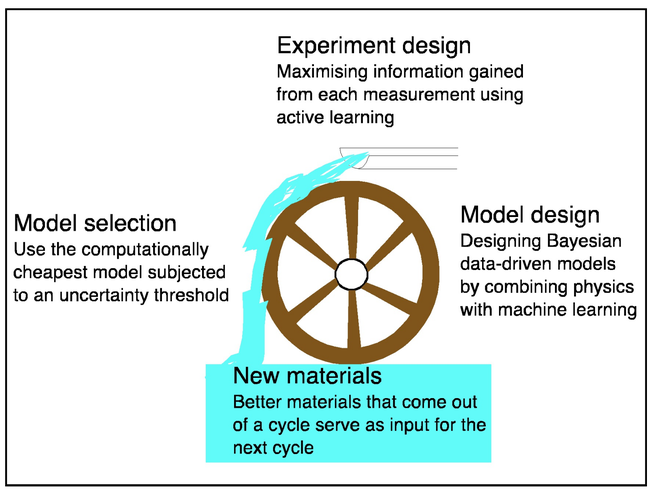
EPSRC Engineering and Physical Sciences Research Council

Designing soft materials using machine learning

Designing molecules to optimize the properties of soft materials such as organic electrolytes and bioactive small molecules is one of the central challenges in materials discovery. We tackle this challenge by combining machine learning with fundamental physics. Some of our current interests include: using unsupervised learning to extract new physics from high throughput simulations and experimental data, designing electrolytes to maximize the capacitance and power of supercapacitors, and realizing an automated workflow for preclinical drug discovery by designing data-driven models that predict the hydration free energy, protein-ligand binding free energy, and synthetic accessibility of organic molecules.

The methodology that we are developing is a three-pronged workflow, combining model selection, model design and experiment design. We develop scalable Bayesian models that can also predict their own uncertainty. The Bayesian approach enables us to go beyond heuristics and develop a statistically optimal method to select between different modelling strategies, balancing between model uncertainty and computational effort. In terms of model design, we design machine learning algorithms that incorporate fundamental physics as inductive bias. Finally, we use an active learning approach to design high-throughput experiments, gaining as much information about the system as possible from the least number of experiments.

Alpha Lee



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