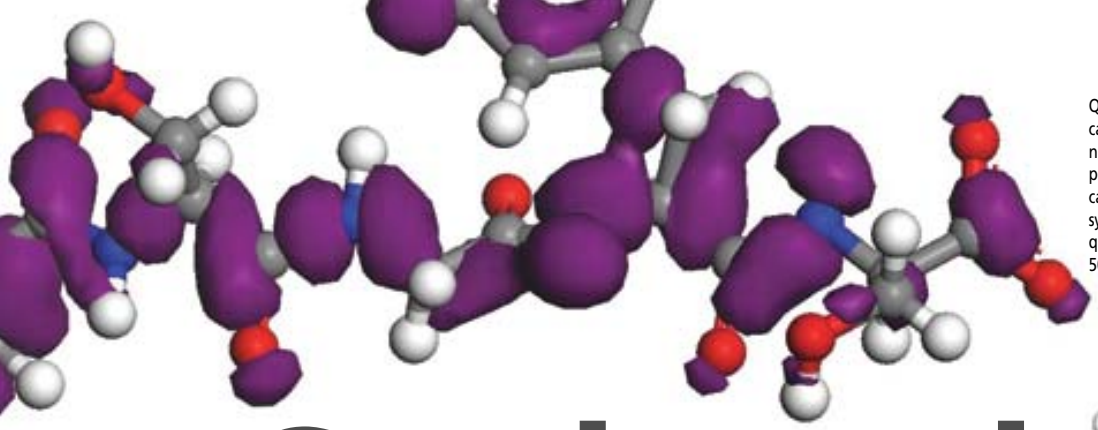
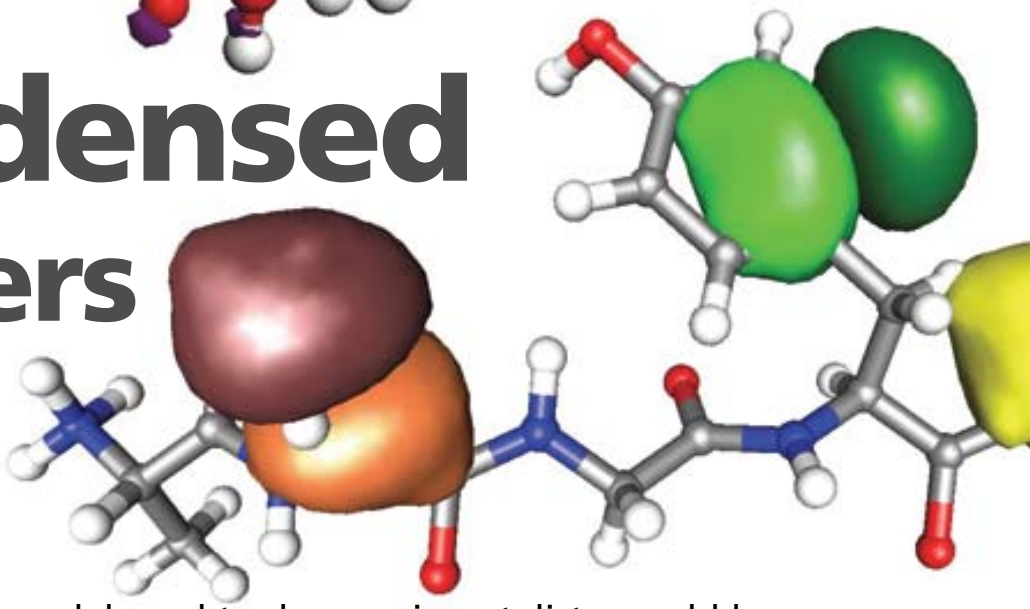


Quantum mechanical calculations generate functions called 'orbitals' which contain all the information necessary for calculating all chemical and physical properties of molecules and solids. Calculations carried out using CASTEP and the new ONETEP system on the same small peptide are equivalent in quality but ONETEP can carry out the calculation on 5000 atoms while CASTEP's limit is about 300 atoms.

Condensed Matters

By David Bradley



Without theories, models and tools experimentalists would be unable to understand what is happening both in the laboratory and in the world around us. *Newsline* talks to the Cambridge scientists who are developing new ways of predicting and modelling the behaviour of matter.

EPSRC's Portfolio Partnerships are aimed squarely at world-leading research teams with a proven track record of ground-breaking science. Through them, EPSRC provides the kind of stable and long-term funding to allow such teams to innovate, explore new research, and establish collaborations with industry and others. The Condensed Matter Group and the Centre for Computational Chemistry at Cambridge University is one such partnership that is benefiting from this inherent stability. With a Portfolio Partnership following on from an EPSRC rolling grant, the Cambridge team has matured into a group with international standing that carries out research at what lead researcher Mike Payne describes as a level above: "We deliver ideas and techniques that lots of other researchers can use, this requires something special!" he enthuses.

"The code would provide a 'virtual laboratory' in which you can carry out any experiment you can think of; experiments that might be very expensive or even impossible in real-life would become possible." Peter Haynes

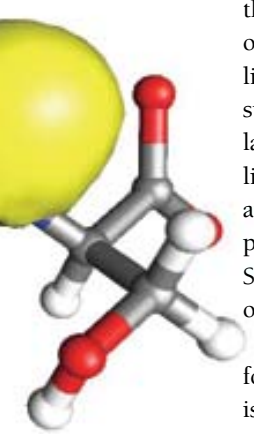
"The Portfolio Partnership cuts us free from the usual round of funding applications," Payne told *Newsline*, "allowing us to be innovative and take risks. If something new comes up, we can change track immediately and chase after it." As such, the scientists within the Portfolio are working on a wide range of research projects – from modelling chemical reactions to understanding superconductivity, and ion transport through narrow pores. They are accessing the behaviour of chemicals at the heart of technologies including drug design and catalysis. Moreover, related mathematical approaches that provide chemists and biologists with new solutions can be applied to cosmological systems and even studies of human aging.

Exotic materials

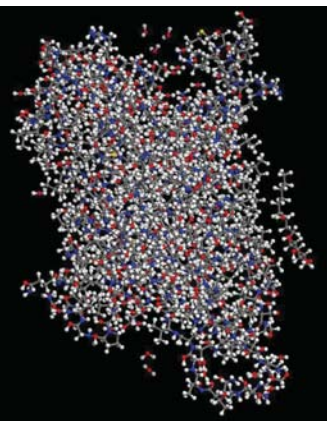
Payne hints that it is in fact very difficult to define specifically the research of the Cambridge team as it is so varied. One colleague, theoretical physicist Mark Warner received the 2003 Agilent Technologies' Europhysics Prize for Outstanding Achievement in Condensed Matter Physics for his work on liquid crystal elastomers carried out with experimentalist colleague Heino Finkelmann and his team at the University of Freiburg in Germany. Liquid crystals are well known in their role in liquid crystal displays (LCDs) on laptops, mobile phones, and digital watches. However, Warner and Finkelmann combined theoretical and experimental work to develop an

Professor Mike Payne (left) and Dr Chris-K Skylaris are hoping to simulate thousands of atoms in a range of systems from water channels to catalyst surfaces.

entirely new class of rubber-like polymers (elastomers) that incorporate the properties of liquid crystals. The resulting unique materials could make them useful in a variety of optoelectronic, telecommunications, and other applications. For instance, liquid crystal elastomers undergo an enormous and reversible stretching when they are warmed and cooled. An equally large effect is obtained on illumination when the elastomer absorbs light, causing them to bend. Further developments of such materials could make them useful as actuators in lab-on-a-chip devices or as artificial muscles. Other liquid crystal elastomers change colour when stretched and could be used to make a new type of laser that can produce any colour depending on the tension applied. Such materials might have applications in optoelectronics and telecommunications.



Work carried out by Jean-Pierre Hansen's team, formerly Rosalind Allen, and now Joachim Dzubiella, is using molecular dynamics to simulate the nanopores that transport water and ions in and out of living cells as well as the kinds of pores found in industrial catalysts, such as zeolites. Results due to appear in the prestigious Journal of Chemical Physics reveal how water permeation controlled by the electric field due to a concentration gradient is coupled to ion transport through a nanopore. The finding will help explain many biological as well as catalytic phenomena seen by experimentalists.

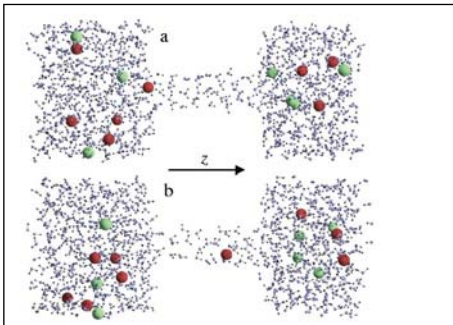


A picture of a 'water channel' showing every individual atom.

A recurrent problem in simulating atomic systems is how to model big systems, such as proteins and catalytic surfaces with limited computer power. Doubling the number of atoms requires eight times the computing power using codes such as Payne's commercial computer package CASTEP. Cambridge researchers would like to circumvent this scaling problem and make quantum simulations scale in a linear way – double the number of atoms and the computing power merely doubles. "Many research groups around the world have attempted this," says Payne, "and there are computer programs that are capable of doing this but with limited accuracy or efficiency." Colleague Peter Haynes and Chris-Kriton Skylaris have been working on an approach to make simulations scale linearly, but without loss of accuracy. Ultimately, the aim is to allow anyone from condensed matter physicists to bench biologists to be able to use a successor to CASTEP to carry out calculations on any atomistic system. "The code would provide a 'virtual laboratory' in which you can carry out any experiment you can think of," Haynes enthuses, "experiments that might be very expensive or even impossible in real-life would become possible."

Nanoscience simulations

For instance, the shape of a protein is crucial to how it works. A biologist can reach inside the protein 'in silico' and alter bond lengths and angles, or add extra chemical groups to the structure. "Identifying the key aspects of the structure can be done much more quickly and cheaply on a computer than in the lab," adds Haynes, "this clearly has huge implications for the development of 'designer drugs'." Chris-Kriton Skylaris and Arash Mostofi are working on the new linear scaling ONETEP code and running simulations on systems with thousands of atoms, such as cellular water channels. "ONETEP can be used to perform highly accurate modelling of such molecules to understand their function at the atomic level," Skylaris told *Newsline*. "The ONETEP method is a 'first principles' approach for quantum mechanical modelling which means that it makes no prior assumptions regarding the properties of the system under investigation," adds Skylaris. The method can therefore be applied to any nanoscience problem, from biology to surface science, which needs an accurate description of the interactions between thousands of atoms, he adds. "The advent of this technique at the same time as the nanoscience revolution is hugely significant," says Haynes, "as technology is becoming increasingly miniaturised, so the scale of systems accessible to quantum-mechanical simulation is increasing and we are entering the era when the scope of these two branches overlap which is tremendously exciting."



Simulation snapshots show how sodium ions pass through a narrow cylindrical pore in the presence of water.

ONETEP is typical of the superb work that is emerging from the Cambridge Portfolio Partnership and represents a discovery with serious practical applications in seemingly disparate research fields. The Portfolio Partnership has played a key role in this development. "How else could one run an eight-year project, fail several times, but still take that sort of strategic view?" asks Payne. ■

Contacts

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