[subject category: Materials]

SUPERCOMPUTERS KEY TO DEVELOPING NEW MATERIALS

Supercomputers will play a key role in developing important new materials of the future that will benefit society, according to theoretical physicists.

For example high-temperature superconductors, in which electricity flows with no resistance, could one day be useful in providing highly efficient power-distribution systems or more efficient medical scanners. However, high-temperature superconductors that have been made so far are ceramics that are brittle and not easy to process. Scientists would like to understand precisely why these materials are superconducting – and then develop more efficient and practical superconductors.

Professor James Annett, a theoretical physicist at the University of Bristol, says, "The materials from which high-temperature superconductors are made are very complex and contain many different types of atom within their crystal structure. The crystals show a surprising level of complexity in their atomic structure, disorder and proximity to magnetism. This makes the system extremely difficult to understand at the atomic scale."

Electric current arises from the flow of electrons. In a superconductor the electrons flow in an unusual way through the crystal lattice. "Electrons are quantum mechanical entities with unpredictable properties," says Professor Annett. "To understand what is happening in a complicated crystalline superconductor you cannot simply look at a single electron, you must work out what is happening to many electrons which are all interacting with each other. These are hugely complicated problems mathematically and expensive computationally."

The availability of a powerful computer such as HECToR will have important implications for materials science, Professor Annett says. "In all these areas there is a key interaction between theory, experiment and computation. Theoreticians such as myself provide experimentalists with new ideas, and they in turn provide us with data to feed into our theories. Computation is a key part of testing our theories and HECToR should help us to make important headway."

-ends-

Contact Professor James Annett. Tel: 0117 928 8752; e-mail: James.annett@bristol.ac.uk