Imperial College London

Doctoral Training Centre

Ten PhD studentships available

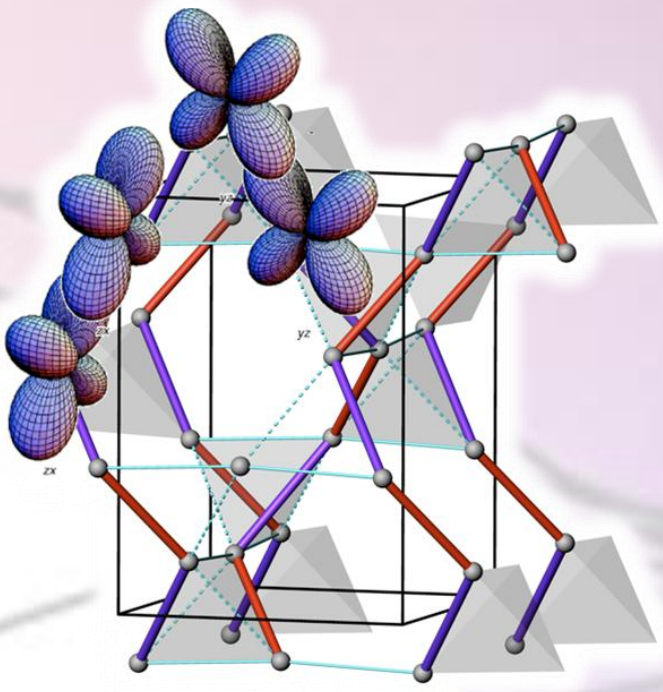
Theory and Simulation of Materials

Do you **relish the challenge** of understanding complex physical phenomena mathematically?

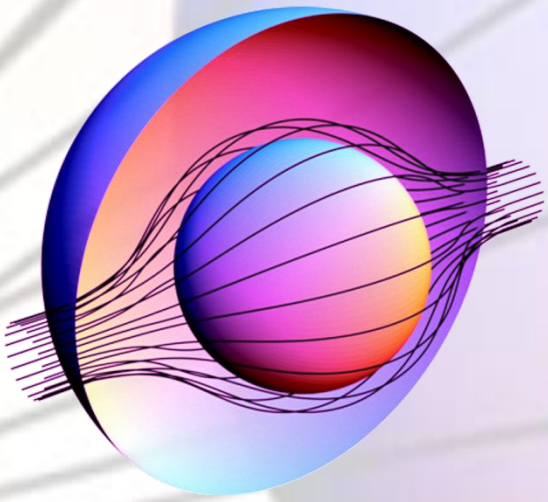
Do you want to apply your **talent for theory** to address the significant issues facing society today?

Modern technology depends vitally on materials: energy generation; telecommunications; aerospace and land transportation; information storage and transmission; healthcare; security and defence.

Theory and simulation are crucial in selecting materials, optimising design and performance, and predicting and avoiding failures. Theory and simulation also free us to **think the unthinkable**: to create entirely new classes of materials e.g. to make objects invisible. This new Doctoral Training Centre (DTC) is about creating new models, new theory and new computational algorithms at the frontiers of materials research.



First-principles quantum-mechanical calculations: Mg-doped TiO_2 forms the cubic $MgTi_2O_4$ phase. The electrons donated by the Mg ion are predicted to localise in particular Ti-*d* orbitals and interact strongly to form an orbitally ordered chiral spin phase which has been observed by neutron diffraction.

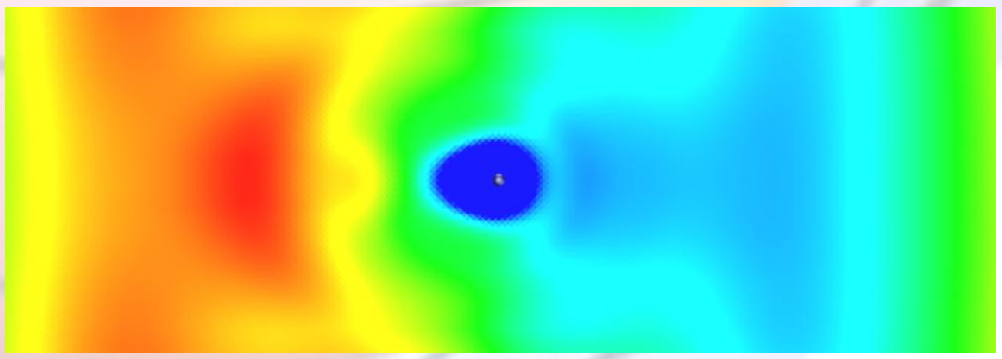


Metamaterials: the optical properties of a material may be tailored by adjusting its microstructure as well as its chemistry. Simulation is used to design such metamaterials, which can even be made to have a negative refractive index. Applications include a perfect lens and an electromagnetic cloak (left).

The **four year programme** combines a taught MSc in theoretical materials physics and simulation techniques, followed by three years of research under two supervisors leading to the PhD degree. The central theme of the DTC is **bridging length and time scales**, which poses some of the most challenging problems in the field.

One of the special features of this DTC is that each intake of students will have a strong sense of **cohort** identity, fostered through group activities, award-winning residential transferable skills courses and a dedicated mentor.

For more information about the course, funding, eligibility and how to apply, visit the DTC web site.



Radiation damage: a 1 MeV ion moves left-to-right down a <100> channel in copper, simulated using time-dependent tight-binding in a simulation cell of 14080+1 ions. Above: the Hartree potential in the plane shows a gradient against the direction of motion, indicating a Coulomb drag force.

EPSRC Engineering and Physical Sciences Research Council

www.cmth.ph.ic.ac.uk/dtc/