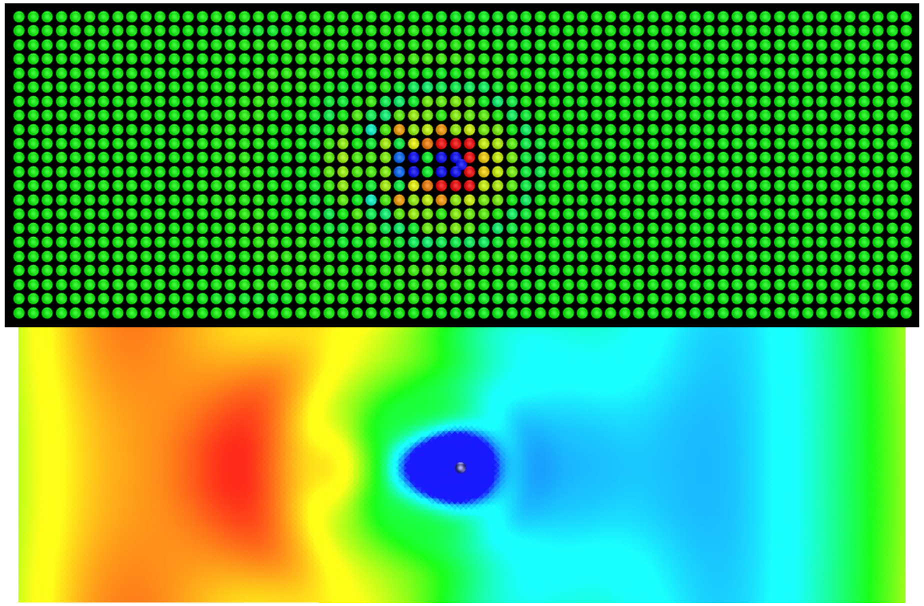
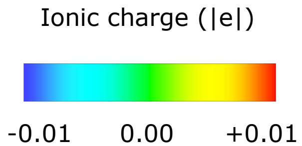




Radiation damage simulation: a 1 MeV ion moves left-to-right down a <100> channel in copper, simulated using time-dependent tight-binding in a simulation cell of 14080+1 ions. Above: the on-site ionic charges show the negatively charged ion is ahead of the compensating screening charge cloud. Below: the Hartree potential in the plane shows a gradient against the direction of motion, indicating a Coulomb drag force.

HOW TO APPLY

Prospective applicants are encouraged to make informal enquiries by contacting the Admissions Tutor Dr Peter Haynes. Applications must be made through the Department of Physics.

Applicants should have, or expect to achieve, a first class Bachelor's or Master’s degree in the physical sciences or engineering. The selection procedure will include an interview with members of the Research Board of the TSM-DTC.

The DTC has funding from the EPSRC for ten four-year PhD studentships per year. This funding may be used to pay the fees of students from the UK and EU, and also the stipends of students who have been "ordinarily resident" in the UK for the last three years.

Applications from students with their own funding are welcomed.

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

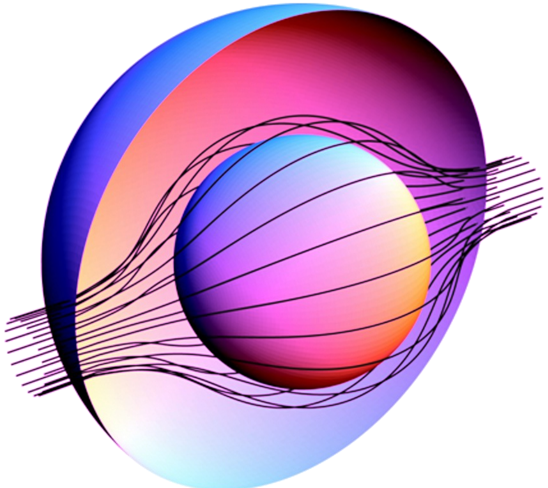
Imperial College London

Doctoral Training Centre

Theory and Simulation of Materials

If you relish the challenge of understanding mathematically complex physical phenomena and processes, and you want to apply your talent for theory to address some of the most significant issues faced by modern society, read on.

It is hard to think of a single modern technology that is not completely dependent on materials. The production of energy, telecommunications, aerospace and land transportation, the storage processing and transmission of information, healthcare, security and defence, and pretty much everything else we take for granted in modern life, are all dependent on materials.



Metamaterials: it has recently been noticed that the optical properties of a material may be tailored by adjusting its microstructure as well as its chemistry. Simulation has been 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, depicted

Our ability to use theory and simulation to guide the selection of materials, to optimize design and performance, and to predict and avoid failures are crucial to all these technologies. Theory and simulation also enable us to think the unthinkable, to create entirely new classes of materials such as materials to render objects invisible.

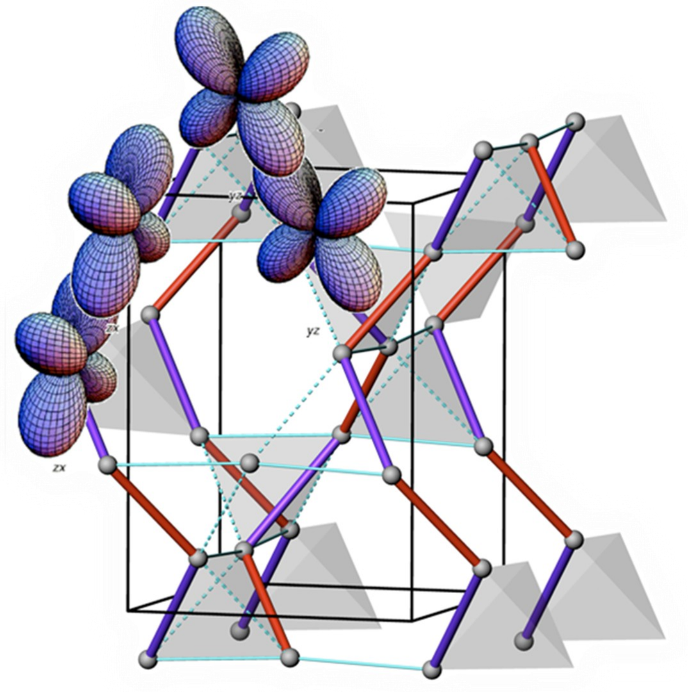
The emphasis in the DTC is on the creation of new models, new theory and new computational algorithms at the frontiers of materials research, as in the surrounding examples. The PhD projects in the Doctoral Training Centre (DTC) will be carried out in the Thomas Young Centre (TYC) which is the London Centre for Theory and Simulation of Materials (TSM).

Supported by: EPSRC Engineering and Physical Sciences Research Council

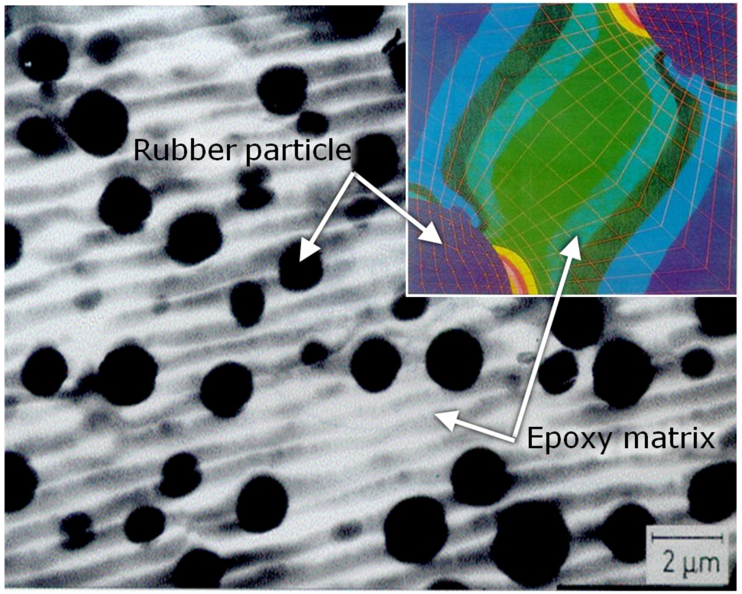
THE DTC EXPERIENCE

This DTC will provide a cutting-edge educational and research environment in TSM across length and time scales, spanning the disciplines of physics, materials, chemistry, aeronautics and chemical and mechanical engineering.

The DTC experience is quite unlike an ordinary PhD. There are student-led seminars and conferences, visiting professors brought in for students to interact with, and several residential transferable skills courses. Students receive not only a unique training and research experience, but also opportunities to explore other aspects of being a scientist or engineer such as leadership, decision making, teamwork and communication. There are also plenty of opportunities to form networks with students, scientists and engineers at other DTCs at Imperial and beyond and in industry.



First-principles quantum-mechanical calculations: when doped with magnesium TiO_2 forms the cubic $MgTi_2O_4$ phase. The electrons donated from the Mg ion are predicted to localise strongly in particular Ti-*d* orbitals. The localised electrons interact strongly to form a beautiful orbitally ordered chiral spin phase which has been observed in neutron diffraction experiments. The bonds distort from the cubic structure to form alternating short (purple) and long (red) bonds due to the alternating orbital occupancy.



Rubber toughened epoxy adhesives: when the material is stressed (e.g. at a crack tip), there will be triaxial tensile stresses acting on the rubber particle due to the different elastic moduli and Poisson ratios of the rubber particle and the matrix. This leads to cavitation of the rubber particles which enables plastic void growth, and hence a large increase in the toughness. Inset: the stress field.

THE MSc COURSE: YEAR 1

The first year is a 12-month, 90-ECTS, Bologna-compliant MSc in the Theory and Simulation of Materials. This course provides a foundation in theoretical materials physics and its applications in simulations across length and time scales.

There are six core courses:

- Mathematical and Computational Methods
- Equilibrium in Materials
- Change in Materials
- Electronic Structure of Materials
- Elasticity and Microplasticity
- Materials Simulation Methods from Electrons to Finite Elements

Students will also select two options in the first year and may take further options in later years. For both the core courses and options, the teaching involves a mix of lectures, directed reading, problem classes, computational exercises and seminars. Assessment is by a combination of coursework and written examinations.