


	<p>Ab Initio Modelling in Solid State Chemistry - MSSC2009</p> <p>http://www.cse.scitech.ac.uk/events/MSSC2009/</p> <p>September 14-18, 2009 - London</p> <p>Directors N M Harrison, G Mallia – Imperial College London</p>	  
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The Department of Chemistry of Imperial College London and the Computational Materials Science Group of the Science and Technology Facilities Council is organizing the tenth MSSC Summer School on the *ab initio* modelling of crystalline and defective solids with the CRYSTAL code. The week long school is designed for new users of CRYSTAL: PhD students, Post-Docs and researchers with interests in solid state chemistry, physics, materials science, surface science, catalysis, magnetism and nano-science. It will provide both an introduction to the capabilities of quantum mechanical simulation and to the practical use of CRYSTAL09 (<http://www.crystal.unito.it>).

Outline of the Subjects

- Basic ingredients in solid state calculations: space groups and point symmetry; reciprocal space and Bloch functions; Hamiltonians and basis sets
- The structure of the CRYSTAL code: selection of the basis set and Hamiltonian; controlling accuracy and numerical precision.
- Parallel execution – exploiting high performance computers
- Total energy and related quantities: equations of state, solid state reactions, phase transitions.
- Geometry optimization: strategies and techniques.
- Vibrational frequencies in solids: lattice dynamics and thermodynamics
- One electron properties: electronic structure, charge, potentials and spin densities
- Surface chemistry and heterogeneous catalysis: models, accuracy and limitations.
- Local defects in solids: the observables of interest; the possible strategies.
- Dielectric properties from CPHF and DFPT.
- Magnetism and properties associated with unpaired electrons.
- Localized crystalline orbitals - Wannier Functions.
- Electron transport

Program

The school will last five days (14-18 September 2009) and will be held at the Chemistry Department at Imperial College London. The course is self-contained with the morning lectures providing the theoretical and computational background required for the afternoon sessions involving practical tutorials. By the end of the week an attentive student will be able to perform reliable calculations of material properties. There will be the possibility to present posters that will be discussed during a special session. Participation is limited to 50 people and participants will be selected from applications received by the deadline. Two registration fees are in operation: £100 for registration only and £375 for registration plus five nights (13-17 September) accommodation at Beit Hall. A small number of bursaries will be available.

Lecturers

The local staff of the Computational Materials Science Group at Imperial College will be joined by international experts from University of Torino (Italy), STFC - Daresbury Laboratory and Rutherford Appleton Laboratory (UK) and MIT - Department of Material Science & Engineering, Cambridge (USA)

Deadlines and Contact Information

The deadline for applications is Friday 24 July 2009. All applicants will be notified of the outcome of the selection process by email during the week commencing Monday 27 July 2009.

E-mail : damian.jones@stfc.ac.uk **Fax:** +44 (0)1925 603634 **Tel:** +44 (0)1925 603805
Postal Address: Damian Jones, MSSC2008, Daresbury Laboratory, Warrington, WA4 4AD, UK