



Ab Initio Modelling in Solid State Chemistry - MSSC2008

<http://www.cse.scitech.ac.uk/events/MSSC2008/>

September 15-19, 2008 - London

Directors

N M Harrison – Imperial College London
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**Imperial College
London**



The Department of Chemistry of Imperial College London, the Computational Materials Science Group of the Science and Technology Facilities Council, and the Department of Chemistry of University College London 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 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 CRYSTAL06 (<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.
- 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: DOS, band structure, charge and spin density maps, electrostatic potential
- 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.
- Explicit electron correlation: MP2 for crystals

Program

The school will last five days (15-19 September 2008) 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 on display for the whole school and discussed during a special session. Participation is limited to 50 people with local accommodation available at Beit Hall in single rooms for £49 per night. The registration fee is £150, which does not include accommodation. A small number of bursaries will be available.

Lecturers

The local staff of the Computational Materials Science Group will be joined by international experts including: M Alfredsson - University of Kent (UK), S Casassa, B Civalleri, R Dovesi, R Orlando, C Roetti - University of Torino (Italy), I Bush, B Searle, A Wander - STFC Daresbury (UK), F Cora - UCL (UK), K Doll - MPI Stuttgart (Germany), CM Zicovich Wilson - Cuernavaca (Mexico)

Deadlines and Contact Information

Registration will close on Friday 15 August 2008 – or before if the limit of 50 people is reached. Poster abstracts must be submitted by Friday 15 August 2008.

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