Ab initio Modeling in Solid State Chemistry

MSSC2007 - *http://www.crystal.unito.it/mssc2007*

September 2-7, 2007 - Torino, Italy

Directors:
B. Civalleri, University of Torino - R. Orlando, University of Eastern Piedmont

The Theoretical Chemistry Group of the Torino University is organizing a new edition of the Summer School on the ab initio simulation of crystalline and defective solids with CRYSTAL. The school is addressed to PhD students, Post-Docs and researchers with interests in solid state chemistry, physics, materials science, surface science, catalysis. It will provide an overview of the possibilities offered by ab initio quantum mechanical techniques when applied to characterize materials.
The new capabilities of CRYSTAL06 (http://www.crystal.unito.it) will be illustrated, with hands-on tutorials organized in the afternoon sections.

Outline of the subjects

- Basic ingredients in solid state: space groups and point symmetry; reciprocal space and Bloch functions; Hamiltonians and basis sets
- The structure of the CRYSTAL code: basis set, Hamiltonian, accuracy.
- 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
- Spin polarized solutions: ferromagnetism and antiferromagnetism, Fermi contact and hyperfine coupling constants.
- Localized crystalline orbitals - Wannier Functions.
- Post-HF ab initio MP2 techniques for crystals
- A special session will be dedicated to answer questions from users

Program

The school will last six days (2-7 September 2007) and will be held at the Chemistry Departments of the University of Torino. The morning sessions will be devoted to lectures by experts. The afternoons will be dedicated to practical sessions. In the tutorials it will be shown how to obtain information concerning various observables using the CRYSTAL code. 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 35 people. Accommodation will be at the University guest house, in single rooms. The total cost of the school is expected to be 780 Euro (650 Euro + 20% taxes). A small number of bursaries will be available, to cover the participation fee of researchers from less favourite countries.

Teachers

The local staff of the Theoretical Chemistry Group will be supported by European scientists, including:

M. Alfredsson, University College (London) - U.K.	Y. Noel, Université P.&M. Curie (Paris) - France
I.J. Bush – CCLRC-CSE (Daresbury) - U.K.	F. Pascale, Université de Nancy - France
M. Catti, Università di Milano Bicocca (Milano) – Italy	M. Rerat, Université de Pau et de l'Adour - France
F. Corà, RI and University College (London) - U.K.	P. Ugliengo, Università di Torino - Italy
K. Doll, MPI (Stuttgart) – Germany	C.M. Zicovich Wilson (Cuernavaca) – Mexico
N.M. Harrison, CCLRC and Imperial College - U.K.	

Deadlines and Contact Information:

Submission of application form: *May 1st* *Notification of acceptance:* *May 15th*
Payment of school fee: *June 5th* *Submission of poster abstracts* *July 15th*

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