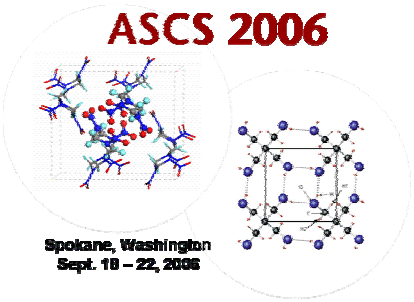

Ab initio Simulation of Crystalline Systems

ASCS2006 - http://www.crystal.unito.it/ascs2006
September 17-22, 2006 - Spokane, Washington, USA
Directors: W. F. Perger, Michigan Tech University
R. Dovesi, University of Torino

The Theoretical Chemistry Group of Torino University, in co-operation with Michigan Tech and Washington State University, is organizing a new edition of the Summer School on the *ab initio* simulation of crystalline systems and solids with defects. The school is addressed to PhD students, Post-docs and researchers with interests in solid-state chemistry, physics, materials science, surface science, and 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: vibrational frequencies and IR intensities at Gamma point, full geometry optimization (atom co-ordinates and cell parameters).

Outline of the subjects:

- **Introductory lectures: 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.**
- **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**
- **Localized crystalline orbitals – Wannier functions**
- **Dielectric properties**
- **Spin polarized solutions: ferromagnetism and antiferromagnetism, Fermi contact and hyperfine coupling constants**
- **Post-Hartree-Fock ab initio MP2 techniques for crystals**
- **A special session will be dedicated to vibrational frequencies in solids: from theory to experiment.**

Program

The school will last 5 days (18-22 September 2006) and will be held at the Ridpath Hotel in Spokane, Washington, USA. 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 entire school and discussed during a special session.

Participation is limited to 35 people. Accommodations will be at the Montvale Hotel. The total cost of the school is expected to be $700. Grants will be available and preference will be extended to PhD candidates and post-docs.

Teachers

The Theoretical Chemistry Group from Torino University in collaboration with scientists from the rest of Europe, the US, and Mexico, including:

M. Catti, Università di Milano Bicocca (Milano) - Italy	**B. Civalleri, Universita' di Torino (Torino) - Italy**
F. Corà, The Royal Institution and University College London - U.K.	**R. Dovesi, Universita' di Torino (Torino) - Italy**
Y. Noel, Université P. et M. Curie (Paris) - France	**R. Orlando, Universita' di Torino (Torino) - Italy**
W. Perger, Michigan Tech University - USA	**C. Roetti, Universita' di Torino (Torino) - Italy**
P. Ugliengo, Universita' di Torino (Torino) - Italy	**C. M. Zicovich Wilson, Universitat Autonoma del Estato de Morelos, Cuernavaca - Mexico**
E. Aprà, Pacific Northwest National Lab - USA	

Deadlines and Contact Information:

Submission of application form: ***June 15th, 2006***
Payment of school fee: ***August 1st, 2006***
Notification of acceptance: ***July 15th, 2006***
Submission of poster abstracts: ***August 1st, 2006***

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