Ab initio Modelling in Solid State Chemistry

MSSC2013

Featuring CRYSTAL13 and CRYSCOR13

http://www.crystal.unito.it/mssc2013

September 1-5, 2013 - Torino, Italy

Director: R. Dovesi (University of Torino)

The Theoretical Chemistry Group of the Torino University is organizing a new edition of the Summer School on the ab initio simulation of crystalline solids. Its aim is to illustrate the new features of CRYSTAL13 (http://www.crystal.unito.it) and CRYSCOR13 (www.cryscor.unito.it) programs. The school is addressed to all CRYSTAL's users, senior researchers and scientists and PhD students with a good background in solid state chemistry and physics, who can take advantage of the new developments for applications to materials science, surface science, catalysis. The new capabilities of the codes will be demonstrated with hands-on tutorials organized in the afternoon sessions.

Outline of the subjects

The theoretical aspects, some implementation details and applications of the new features of CRYSTAL13 will be discussed. These include: calculation of dielectric properties through the CPHF/CPKS scheme: linear (static and dynamic) and non-linear (static, up to the fourth order); Raman intensities; automated calculation of elastic constants and piezoelectric/photoelastic constants; special symmetries (nanotubes and helices) nanostructures and low-dimensionality systems; extension of DFT methods to Double hybrids, Range-separated hybrids, mGGA; enhanced parallel versions of CRYSTAL: Pcrystal and MPPcrystal

A special session will be devoted to post-HF techniques for crystalline systems with the presentation of the CRYSCOR13 program: discussion of the theoretical background, mode of use and recent applications.

Program

The school will last six days (1-5 September 2013) and will be held at the Chemistry Departments of the Torino University. The morning sessions will be devoted to lectures by experts. The afternoons will be dedicated to practical sessions: the tutorials will demonstrate the new features of CRYSTAL13 and illustrate the mode of use of CRYSCOR13. Participants are allowed to present posters which will be on display and discussed during a special session on September 4th.

Participation is limited to 40 people who will be selected among applicants within the deadline. The fee is expected to be 605 Euro (500 Euro + 21% taxes), which includes coffee breaks, lunches and accommodation in double rooms at the University guesthouse. A small number of bursaries will be available.

Teachers

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

E. Aprà, EMSL/PNNL - USA	B. Kirtman, University of California S. Barbara - USA
M. Causà, Università di Napoli - Italy	M. Lorenz, Universität Regensburg - Germany
P. D'Arco, Université P.&M. Curie (Paris) - France	M. Peintinger, University of Bonn - Germany
R. Evarestov, University of S. Petersburgh - Russia	M. Rérat, Université de Pau - France
C. Gatti, Università di Milano Bicocca - Italy	C.M. Zicovich Wilson, Univ. Cuernavaca - Mexico

Workshop in Memory of Cesare Pisani

On September 6-7th, there will be a two-day workshop in memory of Cesare Pisani. Eminent scientists (see http://www.theochem.unito.it/WSSQC-13) will give a survey on several areas of solid state quantum chemistry Cesare Pisani significantly contributed to develop.

Deadlines and Contact Information:

Submission of application form:	*June 15th*	*Notification of acceptance:*	*June 21st*
Payment of school fee:	*July 15th*	*Submission of poster abstracts*	*July 31th*

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