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 CRYSTAL09 (http://www.crystal.unito.it) and CRYSCOR09 (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 CRYSTAL09 will be discussed. These include: advanced geometry optimization tools (e.g. transition state search); phonon dispersion and related properties; automated calculation of the elastic constants and equation of state; calculation of linear and non-linear dielectric properties through the CPHF/CPKS scheme; special symmetries (nanotubes and helices) and nanostructures; combinatorial mapping of solid solutions and magnetic configurations; 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 CRYSCOR09 program: discussion of the theoretical background, mode of use and recent applications.

**Program**

The school will last six days (4-9 September 2011) 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 CRYSTAL09 and illustrate the mode of use of CRYSCOR09. Participants are allowed to present posters which will be on display and discussed during a special session on September 7th.

Participation is limited to 40 people who will be selected among applicants within the deadline. The fee is expected to be 720 Euro (600 Euro + 20% 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:

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<thead>
<tr>
<th>Name</th>
<th>Institution</th>
<th>Country</th>
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<tr>
<td>P. D’Arco</td>
<td>Université P.&amp;M. Curie (Paris) - France</td>
<td>France</td>
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<tr>
<td>M. Catti</td>
<td>Università di Milano Bicocca - Italy</td>
<td>Italy</td>
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<td>M. Schütz</td>
<td>Universität Regensburg - Germany</td>
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<td>D. Usvyat</td>
<td>Universität Regensburg - Germany</td>
<td>Germany</td>
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<td>I. J. Bush – NAG (Oxford) - UK</td>
<td>R. Resta, Università di Trieste - Italy</td>
<td>Italy</td>
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<tr>
<td>K. Doll, MPI Stuttgart - Germany</td>
<td>C.M. Zicovich Wilson, Univ. Cuernavaca - Mexico</td>
<td>Mexico</td>
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**Memorial Carla Roetti**

On September 7th, there will be a day in memory of Carla Roetti. Eminent scientists (E. Clementi, F. Illas, ...) will give a survey on the development of theoretical and computational chemistry from molecules to solids and viceversa.

**Deadlines and Contact Information:**

- **Submission of application form:** June 30th
- **Notification of acceptance:** July 15th
- **Payment of school fee:** July 31st
- **Submission of poster abstracts:** July 29th

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