Prof. Roberto Dovesi

Positions (Universita' degli Studi di Torino) CNR fellowship:1971-1975

Lecturer: 1975-1982

Associate professor: 1983-2000

Full professor: 2000-present

Head of Department of Chemistry IFM: 2009-2011

His scientific activity focuses on the use of a quantum-mechanical approach to solid state chemistry, physics, materials science, surface science. In particular, his primary activity is the implementation of ab initio computer programs for the study of the electronic structure of periodic compounds. The main outcome of this activity is the ab initio CRYSTAL program (study of the electronic structure of systems periodic in 3, 2, 1 and 0 dimensions). CRYSTAL solves both the Hartree-Fock and Kohn-Sham equations, using the LCAO scheme and atom-centred Gaussian basis functions, and provides a full characterization of solids, through the calculation of many properties. It is the result of about 35 years work (1976-2012) by the theoretical chemistry group at the University of Torino (many collaborations, the most relevant with V.R. Saunders since 1982). The theoretical background behind the CRYSTAL code is described in references listed at the web page: http://www.crystal.unito.it/theorframe.html. CRYSTAL06/09 is in use in more than 350 laboratories in the world. For a long period CRYSTAL has been the only public periodic ab initio code available to the scientific community. In December 2013 a new release will be delivered.

The second area of interest of Roberto Dovesi is the application of the CRYSTAL code to surface science and catalysis, geophysics, materials science, solid state chemistry and physics of perfect and defective systems, vibrational, thermodynamic and optical properties of crystalline systems, effect of an electric field on a crystalline solid, nanotubes, solid solutions. Roberto Dovesi is the author of more than 250 papers published in international journals and of one book (with Cesare Pisani and Carla Roetti) published by Springer in 1989. Since 1985, he received more than 7000 citations with h-index=51 (source: ISI Web of Science). In the last five years more than 30 Ph.D students/Post-Docs from European countries visited the Torino theoretical

group for periods of 2-36 months, in order to be introduced to the formal aspects and use of the CRYSTAL code.

Roberto Dovesi organized in 1995 a European summer school in Torino, as part of the activity of a Human Capital and Mobility EEC network with title "Development and Applications of the Hartree-Fock Method in Materials Science", for the implementation and use of the CRYSTAL program (11 laboratories were involved). International schools on ab initio Modeling in Solid State Chemistry (denoted as "MSSC") are periodically organised: 2000, 2001, 2002, 2003, 2006, 2007, 2009, 2011, 2013 (Torino). Similar schools were organized by Roberto Dovesi and collaborators in Pau (FR; 2003), Barcellona (ES; 2004 and 2009), London (UK; 2004, 2008, 2009, 2010, 2011, 2012, 2013), La Plata (Argentina; 2004), Spokane (USA; 2007), Guangzhou (China; 2011), Riviera Maya (Mexico; 2011), Natal (Brazil; 2012). In 2014 two schools will be held in Perth (Australia) and at Bundelkhand University, Jhansi, India (see in the CRYSTAL web-site at the EVENTS entry).