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New information from modern charge density methods

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The charge density (CD) of a chemical compound is probably the most information-rich observable that is available for the system. It contains much information on the chemical bonding as well as on physical and chemical properties. It can be determined experimentally from elaborate diffraction experiments at short wavelength and low temperature. In some cases, it can also be calculated from theory. The CD defines the electronic ground state of a system, and this insight has led to the illustrious successes of the density functional theory in computational chemistry and physics. Owing to its fundamental importance, the CD is used across many disciplines in physics, chemistry, biology and the life sciences. The framework used when discussing the CD may depend on the particular aspects under study, but the fundamental physical observable remains the same.

The present collection of research papers deals with diverse aspects of modern charge-density research. The authors participated in the Third European Charge Density Meeting (ECDM-III), which took place 24–29 June 2003 at Sandbjerg Estate, a conference center owned by the University of Aarhus, Denmark. All contributions were refereed in the normal way.

The CD topic is highly international with strong research groups located all around the globe. Within the community, the tri-annual Sagamore and Gordon Conferences on electron, momentum and spin densities have a long history of vibrant and informative meetings. Nevertheless, suggestions of closer cooperation between European crystallographers interested in electron-density determination matured by the mid-nineties, and the idea of regular European Charge Density Meetings was conceived during the British Crystallographic Association Meeting in December 1995 at Durham University, which featured a special charge-density session with international attendance. The first regular ECDM meeting was held in Nancy in November 1996 and was followed by ECDM-II in Sitges near Barcelona in October 1999. ECDM-III at Sandbjerg Estate was therefore really the fourth in a series of meetings aimed at advancing the craft of electron-density determination and interpretation for use in chemical, physical and biological sciences.

For ECDM-III, we decided to reach out towards different branches of science and applied for funds from the European Science Foundation to run in connection with ECDM-III an Exploratory Workshop with the theme *New information from modern charge density studies*. We are grateful that the European Science Foundation accepted the idea and granted the necessary means to invite about 20 top scientists to attend and lecture, and to engage in stimulating interdisciplinary discussions. ECDM-III thus became a forum at which new directions for future charge-density studies were envisioned and transnational cross-disciplinary networks were formed.

It is also a great pleasure to thank the International Union of Crystallography for sponsoring the participation of a number of young scientists.

In order to highlight the amazing breadth of the CD field, the papers are assigned to three groups. A lead-in essay by Coppens & Volkov gives an overview of the interplay between experiment and theory in CD analysis.

Then follows a group of papers showing the diverse experimental diffraction techniques used in CD analysis stressing the importance of data quality: Destro *et al.* (conventional X-rays), Birkedal *et al.* (synchrotron X-rays), Poulsen *et al.* (synchrotron X-rays), Luger *et al.* (synchrotron X-rays), Jauch (γ rays), Friis *et al.* (electrons), and a paper by Katrusiak on the possibility of CD studies in high-pressure experiments using powder diffraction.

Next follows a group of papers that present new theoretical developments in the interpretation of CD distributions and for calculating molecular and crystal properties. They deal with calculations of electronic and exchange energy density distributions

(Tsirelson & Stash), the topological electrostatic potential (Popelier *et al.*), other topologically defined properties (Luaña *et al.*), the source function (Gatti & Bertini), as well as the effect on the CD of a metal–insulator phase transition (Madsen).

Finally, a group of papers presents a variety of challenging CD studies of interest in physics and chemistry. Molecular magnetic materials (Pillet *et al.*), electric field induced structural and CD modifications (Hansen *et al.*), photoinduced phenomena (Cole), polymorphism (Overgaard & Hibbs), and topological and bond characterization of transition-metal compounds (Wang *et al.*, Marabello *et al.*, Macchi & Sironi and Kožíšek *et al.*).