

SIG#2: “Charge, Spin and Momentum Densities”; report 2006.

SIG#2 has seen a very active 2005 and will see an even more active 2006:

- **IUCr; XX general assembly and conference; Florence, Italy. 23-31 August 2005.** There has been a large and very qualified participation from our SIG members to the various activities of the XX IUCr congress (Florence, August 23-31, 2005). Claude Lecomte (FR), as Chair of IUCr commission on Charge Spin and Momentum Densities (CSMD), was in the Scientific Program Committee and Louis Farrugia (UK), Bo B. Iversen (DK), Nour Eddine Ghermani (FR) and Peter Blaha (Austria) acted as chairs in the 3 microsymposia directly related to the CSMD area (MS 34 : *Advances in Computational Methods for Electron Density Studies*; MS 49 : *Charge, Spin and Momentum Densities in Material Science*; MS 63 : *Chemical Insights from Electron Density Studies and Wavefunctions*). Nine out of the selected fifteen speakers in these 3 MS came from Europe, covering diverse fields of CSMD activities, ranging from the development of computational, methodological and interpretive aspects of charge density (CD) studies (R. Orlando and C. Gatti, IT, B. Guillot and J.M. Gillet, FR), to the high energy synchrotron radiation CD studies in materials science (T. Lippman, Germany), to the interplay between entropy and enthalpy contributions to the free energy as deduced from combined CD studies and rigid-body TLS analyses (A. Ø. Madsen, DK) and to CD studies of highly debated chemical issues (P. Luger and D. Stalke, Germany; A. Korlyukov, Russia). Even more importantly, SIG members have been appreciated speakers in other interdisciplinary MS, denoting that our field is certainly not crystallized but one experiencing a fast internal evolution. K. H. Schwarz (Austria) gave a lecture in MS 10 *Integrated crystallography, spectroscopic and computational approaches*, B. Gillon (FR) and M. Y. Antipin (Russia) in MS 24 *Molecular Crystals under non ambient conditions*, W. Scherer (Germany) in MS 59 *Application of synchrotron and neutron facilities in structural chemistry*, S. van Smaalen (Germany) in MS83 *Computational problems and solutions for aperiodic crystals*. R. Dovesi (IT), one of the main authors of the CRYSTAL-XX series of codes, which are largely used and promoted within our SIG, gave a keynote lecture illustrating the recent progresses in the computation and analysis of vibrational properties of crystalline materials; V. Tsirelson (Russia) chaired the keynote lecture delivered by M. Spackmann. More than 60, highly visited and discussed posters have been presented in about 8 sections, variously related with the SIG activities. Contribution from the European component has been impressive.
- **A new “priority program”** by the “Deutsche Forschungsgemeinschaft”, entitled: „Experimental charge densities for better understanding of chemical interaction“ (SPP1178), shows the strength of the German charge density community. It has started in May 2005 and is supporting about 30 groups, most of them involved in SIG#2.

- **4th European Charge Density Meeting, Brandenburg, 26.- 29.01.2006:** The 4th European Charge Density Meeting was organized by the group of Ullrich Pietsch (Potsdam, later Siegen) and took place in Germany for the first time. It received high acceptance by European charge density community. Ten high ranking scientists accepted the invitation to report about actual developments in experimental and theoretical charge density analysis by invited talks. There are electron localization in organo-metallic compounds (Scherer), light-induced metastable states (Pillet), photoisomerization (Cole), evaluation of thermodynamic values from x-ray data (Madsen), or ELF topology (Silvi), extension of the program code CRYSTAL (Civalleri) or new developments based on density functional theory (Rosner). The program was completed by additional 16 oral talks and 21 posters. Fortunately 37 from total 96 participants were students contributing by talks and discussion to the success of the conference. Considering the large number of students the conference program has included two tutorial talks (Luger, Stalke) in the beginning. The conference took place in Bollmannsruh a pleasant place near Beetzsee in Brandenburg. Nice but cold weather and perfect organization were the basic for success of the conference.
- **The 5th European Charge Density Meeting** will be organised in Italy by Carlo Gatti and Piero Macchi and R. Destro (Milano). In conjunction with this, the organisers will apply for European Funding (COST).
- **ECM-23 Leuven Belgium** (August 7-10, 2006). SIG#2 organises two micro symposia: MS42 – “Structure-property relationships in molecular crystals” and MS13 – “Understanding molecular interactions” (Jointly with SIG#7). SIG#2 also provides one plenary lecture by: Ludwik Dobrzynski. Due to the Sagamore conference in the following week, participation of the SIG#2 community to the ECM23 will be lower than usual.
- SIG#2 is heavily involved in the organisation and participation of the **“Sagamore” conference on Charge, Spin and Momentum density.** Organised by Prof. Malcom Cooper and held from the 13th till the 18th August 2006 in Warwick, England. The Sagamore is together with the Gordon Conference the major conference of the community.
- Gordon conference on chemical bonding 2007 is now scheduled for July 1-6 2007, Mount Holyoke College. Carlo Gatti will act as chair and D. Jayatilaka as a co-chair. Large involvement of SIG#2 members is usual at this Gordon conference.