

SIG #2: charge, spin and momentum densities, Report of 2004 and preview of 2005.

Chair: Heinz Graafsma

Vice chair: Ulrich Pietsch

Secretary: Carlo Gatti

Scientific Meetings:

In 2004 two major meetings were organised with the involvement of SIG #2.

1. ECM-22; Budapest, 26-31 August 2004. A Plenary lecture was given by Prof. U. Pietsch on: "Electron density determinations under non-ambient conditions". Also two micro-symposia were organised: "Electronic effects in molecular interactions", jointly with SIG #7, and "Electron densities in complex systems and under non-ambient conditions". Both symposia had prominent speakers and were very well attended, just like the plenary lecture, showing the healthy interest in density research in Europe.
2. The Gordon Research Conference (GRC) on *Electron distribution and chemical bonding. The Chemical Bond : densities and dynamics*; Mount Holyoke College, MA, USA, July 4-9, 2004. Chair: John Spence (USA); co-chair: C. Gatti (Italy). This GRC is along with the Sagamore conference one of the major activities of the Charge, Spin and Momentum Densities community and it is traditionally focussed more on the Charge Density aspects and on the chemical features derived thereof. The conference included sessions on thermoelectric materials, electron diffraction, resonant scattering, electron density topology, progresses in charge density refinement, time-resolved crystallography, surfaces, in addition to two exciting poster sessions, each one lasting for two whole days. The conference has been well attended (96 delegates), with large participation from young scientists (55% below 40's) and with prominent attendance from SIG-2, with 55% of delegates and 58% of the invited speakers coming from Europe. Carlo Gatti (Italy) and Dylan Jayatilaka (Australia) have been appointed as the next chair and co-chair, respectively, for the upcoming 2007 GRC.

SIG #2 is involved in or in charge of organising various meetings in 2005 and 2006.

- 1) Members of our SIG, as members or Chair (Claude Lecomte, Nancy) of the IUCr commission on Charge Spin and Momentum Densities, have been highly involved with the organization of the scientific activities in the SIG area for the XX IUCr congress (Florence, August 23-31, 2005). Three micro-symposia (MS), with four out of the six appointed chairs coming from Europe, have been planned plus one keynote lecture:
 - MS 34 : *Advances in Computational Methods for Electron Density Studies* (Chairs: Louis Farrugia and Tibor Koritsanzky)
 - MS 49 : *Charge, Spin and Momentum Densities in Material Science* (Chairs: John Spence, Bo B. Iversen)
 - MS 63 : *Chemical Insights from Electron Density Studies and Wavefunctions* (Chairs: Nour Eddine Ghermani, Peter Blaha)

- A keynote lecture on *Electrostatic and related properties from accurate charge density analysis* will be delivered by Marck Spackman (Perth, Australia), with Vladimir Tsirelson (Moscow, Russia) acting as Chair.
- 2) The fourth European Charge Density Meeting will be held in Brandenburg/Havel 24.-29 January 2006 and organized by Ulli Pietsch and his group from University of Postdam, Germany. The international conference will be partially shared with annual report meeting of German Priority Program "Experimental electron densities as key tool for the understanding of chemical interactions" (see below). In summary we expect 100 to 120 participants both experienced European scientists and students and post-docs. The conference will deal with new trends in charge density analysis and interpretation, including a tutorial program for young students and young scientist.
 - 3) Sagamore XV, 13-18 August 2006. The Sagamore conference is one of the major conferences of the Charge, Spin and Momentum Density Community. The 2006 meeting is organised by Prof. Malcolm Cooper and will be held at Bosworth Hall Hotel in Leicestershire, UK. The conference will cover a broad range of topics of interest to the physics, chemistry and crystallographic community addressed by charge, spin and momentum density studies. For further information see www.sagamore2006.com
 - 4) ECM-23 Leuven, 6-11 August 2006. The chair of SIG#2 is involved in the early stages of putting together the scientific program.

Other activities

In April 2005 about 30 groups received funding by German Funding Agency (DFG) after approval of the new scientific priority program (SPP1178) "Experimental electron densities as key tool to understand chemical interaction". In addition to mainly German groups the funding includes one project of a non-German proposer (Tibor Koricanisky). The total duration of SPP is scheduled for 6 years where each proposal becomes reviewed every 2 years. The major activity of SPP is an annual report meetings (see above). (<http://www.dfg-spp1178.de/>).