

SIG#2: Charge Spin and Momentum Densities

Reported Period: 1 July 2006 - 30 June 2007

Report Date: 30 June 2007

Reported by: Bo Iversen(chair), Ulrich Pietsch(co-chair) and Carlo Gatti(secretary)

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SIG Officers (updated list) :

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1. Introduction.

(50 words max.)

Since November 2006, Bo Iversen (Aarhus University) has replaced Heinz Graafsma (ESRF) as SIG#2 chair. We are continuing to promote activities aimed at increasing and diffusing the interest towards the information that chemists, physicists, biologists and materials science researchers may derive from (combined) charge, spin and momentum density studies

2. Past Activities.

Title: **ECM-23** (August 7-10, 2006)

Number of Participants: about 60 from the CSMD community

Sponsors/Organizers: ECA

Short Description: SIG#2 was in charge of two micro symposia: MS42 – “Structure-property relationships in molecular crystals” and MS13 – “Understanding molecular interactions” (Jointly with SIG#7). SIG#2 has also provided one plenary lecture by: Ludwik Dobrzynski. Due to the Sagamore conference in the week following ECM-23, participation of the SIG#2 community to the ECM23 has been lower than usual.

Title: **Sagamore XV** Conference on Electron, Charge and Spin Momentum Densities, (August 7-10, 2006)

Number of Participants: about 100

Sponsors/Organizers: IUCr, BCA (British Crystallographic Association), EPSRC (Engineering and Physical Sciences Research Council), Warwick University, IOP (Institute of Physics), Daresbury Laboratories and several industries.

Short Description: Members of this SIG have been particularly active in this conference, at various levels. They have served in the Scientific Program Committee (C. Gatti, N. Hansen, J. Howard, S. Larsen), in the International Advisory Committee (B. Iversen, C. Lecomte, F. Sacchetti, V. Tsirelson) and as speakers (M. Hakkala, B. Guillot, R. Destro, P. Dominiak, B. Dittrich, C. Dallera, C. Gatti, M. Kohout, M. Blanco, W. Jauch, W. Scherer, C. Lecomte, C. Lehmann, G. Louprias) or session chairs/co-chairs (J.M. Gillet, S. Larsen, P. Macchi, P. Becker). The conference has shown a strong interaction among the different components of CSMD community and has therefore served to the scope of this meeting.

Title: **DFG SPP-1178 (2005-2011)**

Number of Participants: about 30 groups

Sponsors/Organizers: DFG

This priority programme of the Deutsche Forschungsgemeinschaft, entitled : "Experimental charge densities for better understanding of chemical interactions" is entering in its third year, after a positive judgement from international referees of its activity in the first two years. The program is aimed at diffusing and fostering cutting-edge charge density research among chemists and physicists. SIG#2 members are taking active part in this programme either directly or through its supervision as external international referees. The program shows the strength of the German charge density community and it is carefully monitored by this SIG, also in view of the proposal of a similar program at an European level in the future.

3. Future/Programmed Activities.

Title: Gordon Research Conference (GRC) on Electron Distribution and Chemical Bonding: Dynamics and Densities (1-6 July 2007), Mount Holyoke College, USA
Sponsors/Organizers: GRC, NIH (National Institute of Health), IUCr, industries
Short Description: C. Gatti (SIG#2) is acting as a chair and D. Jayatilaka as a co-chair. Large emphasis on time-dependent XRD, XFEL developments, biological aspects of CD research and data quality for CD studies has been given. Participation from Europe seems to be impressive (49 over a total of 99 registered attendees).

Title: Workshop on XD2006 program package: advanced methods in X-ray Charge Density Analysis: Extracting Properties from a Multipole Refinement , September 3-6 2007, Martina Franca (Italy)
Sponsors/Organizers: IUCr, AIC (Associazione Italiana Crystallografia), BCA (British Crystallographic Association), XD-group, INSTM and several industries
Short Description: The new version of XD-2006 will be presented, along with cutting-edge applications and developments in CD studies. P. Macchi is the chair of the Organizing Committee and 3 members of SIG#2 are in the scientific committee (Gatti, Iversen, Scherer). Participation from Europe is expected to be numerous.

Title: ECM-24 (Marrakech, Maroc, 22-27 August 2007)
Sponsors/Organizers: ECA
Short Description: Three SIGs will be organized by SIG#2 with emphasis on CD studies for coordination chemistry, on the insights in materials science from combined CSMD studies and on new theoretical and experimental approaches for understanding atomic interactions.

Title : ECDM-V (European Charge Density Meeting, June 2008)
Sponsors/Organizers: sponsors to be defined; organizers: at the moment C. Gatti and P. Macchi
Short Description : it should be held on the Lake of Como, Italy, in Gravedona, in the period 6-12 June. A special permission from the organizing Committee of OSAKA-2008 IUCr XXIII General Congress has been already obtained to allow IUCR support, despite the time proximity of ECDM-V with Osaka's meeting. The organizers are currently investigating the possibility to join ECDM-V with the annual meeting of SPP-1178 DFG program (see above)

Title : 2008 IUCr XXIII General Congress, Osaka (Japan, 23-31 August)
Sponsors/Organizers: IUCr

Short Description : Members of SIG#2, as also members of the IUCr CSMD commission have been very active in making proposals for key-note lectures and MS titles and chairs. Final decisions will be clearly taken by the International Program Committee.

4. Other matters.

(50 words max.)

Supplementary Materials : no supplementary material

(List of all supplementary materials, if any, related to the SIG report)

- Addendum 1 (to be sent in separate files)
- Addendum 2 (to be sent in separate files)
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- Addendum n (to be sent in separate files)

NOTE: DO NOT FORGET TO SEND THE UPDATED LIST OF YOUR SIG OFFICERS

see above!