

## **Minutes of the IUCr-CSMD open Commission meeting in Madrid (August 27, 2011)**

The CSMD open commission meeting gathered around 30 participants.

From the commission were present: E. Espinosa (new member), C. Gatti (chair), B. Gillon (incoming chair), D. Jayatilaka, U. Pietsch, Y. Sakurai, M. Takata, T. Fernandez-Diaz (ex-officio member, chair of the commission on Neutron Scattering), B. Iversen (leaving-member), M. Spackman (consultant), Y. Wang (consultant) and C. Lecomte (consultant and member of the IUCr executive committee).

C. Gatti (chair) first reported on the composition of the new commission for 2011-2014 and on the recommendations from the IUCr Executive Committee:

- the new members proposed by the commission were accepted by the EC with a restriction about the gender balance which has to be improved for the next triennium (2014-2017)

- two additional consultants were required by the EC: V. Tsirelson and one member of the Commission of Structural Chemistry (to be designated by the SC commission). One member of our commission must be chosen as consultant in the SC commission as well (E. Espinosa was suggested and is willing).

- our commission should be less “closed” and open itself towards biology, structural chemistry, chemical engineering, material science (M. Spackman pointed out that efforts have already been made and are pursued)

- the CSMD commission must contribute to the online dictionary. C. Lecomte precised that almost no terms specific to our commission are included at present.

- two new CSMD projects were suggested by EC: - round-Robin test on a small molecule from data of different large-scale facilities in conjunction with SR commission; - comparison of CD database on a (large) biological molecule.

- required production from the commission: one feature article in Acta B and a basic book in the IUCr series

- International Year of Crystallography in 2013: actions in coordination with the other commissions are required.

Recent information on the upcoming conferences for 2012 was given by their organizers (or representative):

- The location and tentative topics of the Sagamore XVII conference (15-20 July 2012, Hokkaido) were presented by M. Takata. The conference will be hosted by RIKEN Spring-8 Center and co-hosted by several light sources and neutron facilities in Japan and Taiwan as well as Tohoku electron microscopy center. The theme of Sagamore XVII will be «Great Potentials from Advanced Probes». It will take place in a hotel at Lake Toja in Hokkaido; two other hotels only (slightly less expensive) can be found in the neighborhood.

The expected registration fees (including full accommodation) are 1500\$ for regular participant and 1200\$ for students (prices are not guaranteed because of foreign exchange). C. Lecomte pointed out that expected IUCr fundings will not exceed 4000\$. It was asked to separate the registration fees from the accommodation fees but M. Takata explained that the present arrangement ensures the best prices.

- J. Kozisek presented the first announcement of ECDM26 (High Tatras, Slovakia, 16-19 Sept. 2012). Registration fees are moderate (early registration 290 euros /190 for juniors) and accommodation is cheap (single/shared: 54/36.50 euros per night). A special offer from Springer could be used to publish a book of proceedings. C. Lecomte pointed out that the book should preferably be published by IUCr if funds from IUCr are requested.

Suggestions were solicited from the audience for sessions/microsymposia for Sagamore XVII and ECM27 Bergen. Additional suggestions after the open commission meeting were done by mail (B. Dittrich and C. Gatti). The following themes were proposed:

- Multi-techniques approach
- Structure-function relationships from charge density studies
- Interplay of dynamic processes and electron density
- Comparing theory and experiment (descriptors for experimental electron densities, CCSMD project on constrained wavefunction)
- New directions in data refinement
- Charge density for challenging situations (difficult or exotic cases like high pressure)

A. Bansil reported on the status of the organisation of the next IXS-2013 meeting. The decision between two possible locations in US the will be taken before the end of the year.

The status of the ongoing and future commission projects of the commission was described. D. Jayatilaka presented his report (to be published in Acta Cryst.) on the project on constrained wavefunction which was involving seven groups since 2005.

Among the tentative projects which were suggested at the last GRC2010 commission meeting, only the project on electron density in a target material by quantitative convergent beam electron diffraction (QCBED) and ab-initio computations of solids is materializing thanks to P. Nakashima, who shortly presented prospective ideas.

The suggestions for IYCr 2013 actions to which the CSMD commission could participate were summarized by B. Gillon; some additional ideas have been suggested by the audience:

- organization of crossed sessions between GRC2013 and IXS 2013
- production of a video (or DVD or pdf file) on CCSMD activities
- introduction to large facilities: why, where, when and how?
- on-line exhibitions on Crystallography and Materials, - and Magnetism, - and Pharmacy, - and Biology
- satellite workshop on crystallography at the next International Neutron Scattering Conference in 2013 (proposed by the Commission on Neutron Scattering)
- introduce the 'Laue' name in the GRC2013 subtitle, in honor of IYCr

Finally, the creation of a IUCr Working Group on diffraction data deposition was announced (message from J.R. Helliwell). The specific needs of our community must be communicated to this group, i.e. which type of raw data we would like to deposit/find (for example flipping ratios in PND). A formal workshop on this matter will be held next year at the occasion of one of the crystallography meetings (ACA, ECM or AsCA).

For the commission: B. Gillon (chair) 27/08/2011