

Minutes of the IUCr-CSMD closed Commission meeting - Sagamore XVII (July 17, 2012)- Hokkaido (Japan)

Were present:

Members: J.M. Gillet, B. Gillon, Y. Sakurai, M. Takata

Consultants: C. Gatti, C. Lecomte, Y. Pei, W. Scherer

a) Meetings in 2013:

Two workshops have received the support of the Commission for financial requests from IUCr:

- Synchrotron charge density workshop at APS, organized by Yu-Sheng Chen (ChemMatCar) in March 2013
- Workshop on Resonant Elastic X-ray Scattering in Condensed Matter, 15-19 July 2013 Oxford, England (UK), organized by S. P. Collins, Diamond Light Source.

The progress of the organization of the next Gordon Conference **GRC 2013**, "Pushing the Limits of Experimental and Theoretical Charge and Spin Density Studies" (chair: P. Macchi, co-chair: W. Scherer) were reported by W. Scherer.

The date and place of the next international Conference on Inelastic Xray Scattering **IXS2013**, was communicated by Prof. A. Bansil: 11 – 16 August 2013, Stanford, San Francisco (USA); Organizer: C.C. Kao (SLAC).

b) Conferences and schools to be organized by the Commission in the next triennial:

- The candidature presented by Carlo Gatti for organizing the next Sagamore conference was accepted by the Committee. The location will be near the Como Lake in Italy, easily reachable from Milano Int. Airport. The date could be in 2015 or 2016 in order to avoid conflict with the Gordon Conference which becomes biannual after 2013. September is a favourable period for getting moderate accommodation costs.
- Claude Lecomte announced that an international school on charge and spin densities will be organized by M. Souhassou (Nancy) at the beginning of 2014 at the occasion of the International Year of Crystallography.

c) Commission projects:

- The final report on the project on constrained wavefunction (D. Jayatilaka) was not yet available.
- Project on the study of metallic bonds by QCBED and Xray diffraction.

The proposal sent by Philip Nakashima to the chair (BG) before the Commission meeting was discussed. Wolfgang Scherer is involved in a similar german project and expressed his willingness for taking part to the commission project. Carlo Gatti is interested to collaborate with Philip Nakashima on some of the theoretical aspects which are not detailed in the written project. Yu Pei suggested that the chair (BG) contacts Prof. Kenji Tsuda, from Tohoku Univ., who was attending the Sagamore Conference.

- Round robin test on SR charge density studies on a small molecule

It was decided to perform this round robin test on a molecule-based compound, manganese formate dihydrate, $\text{Mn}(\text{HCOO})_2(\text{H}_2\text{O})_2$, for which several data collections on different SR beamlines (APS, Desy) and conventional Xray source are already available from Bo Iversen who agrees to share his data for this project.

M. Takata and C. Lecomte proposed to perform new data collections on this compound at Spring8 and Soleil respectively.

d) **IUCr on line dictionary**

A few volunteers accepted to write definitions for the dictionary: - momentum density (J.M. Gillet and Y. Sakurai), - charge density (C. Lecomte) and charge density topology (C. Gatti) - magnetization density (B. Gillon)

e) **International Year of Crystallography 2014**

The chair (BG) recalled that the commission is expected to realize some actions and/or productions in the frame of IYCr2014. The suggestions made last year are still valid and any new idea will be welcome:

- setting up of a website where anyone could ask for help in determining charge density
- on-line virtual exhibitions on Crystallography and Materials, - and Magnetism, - and Pharmacy, - and Biology, etc...
- production of a video (or DVD or pdf file) on CCSMD activities

17/07/2012,

For the commission: B. Gillon (chair)