SIG No: 4 Reported Period: 2016-2017 Report Date: 30.06.2017 Reported by: Mauro GEMMI

#### 1. Introduction.

The aim of SIG#4 is to raise the awareness and acceptance of Electron Crystallography to a rank comparable to X-ray crystallography. Last achievements of the community are: use of electron diffraction data for structure refinement and identification of hydrogen, application of electron diffraction tomography to protein crystallography

#### 2. SIG web site:

SIG 4 url: https://ecaelectronsig.wordpress.com/

# 3. Number of ECA individual members registered with the SIG according to<br/>(http://www.xray.cz/eca/im-payment.htm)SIG 4electron crystallography120

4. Existence of a SIG mailing list X Yes / O No Address of the mailing list: ecaelectronsig@iucr.org Number of members in the SIG mailing list : 45

## **5.** Approximate total number of researchers involved in the SIG (please indicate the basis for the estimate)

45 researchers (mailing list)

#### 6. List of MS organized by the SIG at the last ECM

- MS27 Dynamical refinement of electron diffraction data
- MS28 New approaches in electron crystallography

#### 7. Prizes sponsored/coordinated

We coordinated two poster prizes on electron crystallography sponsored by Calidris and Nanomegas respectively.

#### 8. Past Activities other than Microsymposia at ECM

#### Title: Electorn crystallography school, September 18-24, 2016, Beijing

Number of participants: 83

Level of involvement of SIG in the activity:

- ECA Individual Members registered with the SIG involved in the organizing committee
- ECA Individual Members registered with the SIG involved as lecturers

Financial support by ECA: no

Short Description: The workshop was held at Peking University and organized by Junliang Sun via Chinese Crystallograhy Society and Peking University. Junliang Sun, Wei Wan and Xiaodong Zou from Stockholm University were the lecutrers. This course covers fundamental crystallography and electron microscopy, structural analysis using electron crystallography, and its combination with powder X-ray diffraction to solve complex structural problems. It includes lectures followed by practical sessions.

#### Title: **ED-XPD Workshop - Combining Electron and X-ray Powder Diffraction Techniques for Structural Characterization**, June 6-10, 2016 Stockholm, Sweden

Number of Participants: 52

Level of involvement of SIG in the activity:

- ECA Individual Members registered with the SIG involved in the organizing committee
- ECA Individual Members registered with the SIG involved as lecturers

Sponsored by ECA: no but supported by IUCr.

Short Description: The workshop was held at Stockholm University and organized by Lynne McCukser, Wei Wan and Xiaodong Zou. The purpose was to combine electron diffraction and X-ray powder diffraction to characterize the structures of polycrystalline materials. It includes lectures followed by practical sessions. 51 people from 14 countries, including 5 lecturers and 9 assistants participated in the workshop.

### Title: International School on Fundamental Crystallography with applications to Electron

**Crystallography** (1 week school, 27 june – 2 July 2016, at University of Antwerp) Number of Participants: 41 (38 students, 3 lecturers)

Level of involvement of SIG in the activity:

- ECA Individual Members registered with the SIG involved in the organizing committee
- ECA Individual Members registered with the SIG involved as lecturers

The School was sponsored by ECA with a 1000 Euros for travel grants for the students Short Description:

The school intended to give the participants a basic knowledge in crystallography, as well as how to use it in the context of a transmission electron microscope. The school focussed on basic knowledge of electron diffraction patterns and on the crystallographic information that could be obtained from such patterns.

Title: International School on Fundamental and Electron Crystallography (IASFEC'2017) will be held on 8 to 13 of October 2017 in Sofia, Bulgaria

Number of participants: 40

Level of involvement of SIG in the activity:

- SIG members involved in the organization
- ECA Individual Members registered with the SIG involved as lecturers

Financial support by ECA: yes

Short Description: The School is organized by the Bulgarian Crystallographic Society with the Support of SIG4 on Electron Crystallography and with the financial support from: ECA, IUCr and National Science Fund of Bulgaria. The school has two parts : a part on general crystallography and a second part totally dedicated to crystallographic application of electron diffraction.

## Title: AIC International School 2017 Bridging the gap between cryoEM and crystallography September 3-6 2017 Pavia, Italy.

Number of Participants: 100

- ECA Individual Members registered with the SIG involved in the organizing committee
- ECA Individual Members registered with the SIG involved as lecturers

The school is sponsored by IUCr

The school is intended to touch all the experimental and computational aspects that are beyond the use of cryoEM for solving the structure of macromolecules.

Title: **Workshop on 3D electron crystallography for macromolecular compounds** September 18-22 2017 PSI Villigen Switzerland. Number of participants: 40 Level of involvement of SIG in the activity:

- SIG members involved in the organization
- ECA Individual Members registered with the SIG involved as lecturers

Financial support by ECA: No

Short Description: This workshop addresses crystallographers in the field of structural biology who want to expand their knowledge to electron crystallography. The list of speakers encompasses experts in sample preparation, electron microscopy hardware, electron detectors, and methods from data processing, structure solution to model building.

Title: Workshop on Electron diffraction for materials science and pharmaceutical applications 21<sup>st</sup> of August 2017 PSI Hyderabad India, during the 24<sup>th</sup> IUCr Congress.

Number of participants: 40

Level of involvement of SIG in the activity:

- SIG members involved in the organization
- ECA Individual Members registered with the SIG involved as lecturers

Financial support by ECA: No

Short Description: This workshop is focused on application of electron diffraction to materials science and pharmaceutical and it is specially designed both for people of academia and industry that, coming from completely different field, would like to expand their knowledge to electron diffraction and imaging.

Several SIG members are involved in the organization of microsimposia for the 24<sup>th</sup> IUCr congress in Hyderabad India.

#### 9. Future/Programmed Activities.

Next year several SIG members will be involved in the organization of the Electron Crystallography school that will be held in Erice.

Title: **51<sup>st</sup> International School of Crystallography on Electron Crystallography** June 2018 Erice Italy.

#### **10. Other matters.**

Our representative for the ECM31 in Oviedo Enrico Mugnaioli has already contacted other SIG representatives and the organizers of ECM31 for the organization of the microsymposia proposed and supported by the SIG4. The SIG4 has proposed the following microsymposia:

- 1) Advances in electron crystallography methods
- 2) Advances in electron crystallography methods in collaboration with SIG01
- 3) Electron crystallography methods for structure characterization of small molecule organic and hybrid materials in collaboration with SIG13
- 4) Experimental methods and computer modelling for defects and disorder quantification at the nanoscale in collaboration with SIG09
- 5) Combined approaches for structure characterization of functional materials in collaboration with SIG05 and SIG12
- 6) Combined approaches for structure characterization of modulated and complex structures in collaboration with SIG05 and SIG12
- 7) Mineralogy at the nanoscale: from nature to applications in collaboration with SIG 05

The SIG4 has also proposed his member Lukas Palatinus for a keynote lecture.

#### **11. Brief annual activity report**

SIG#4 is always very active in organizing school to teach young crystallographers about the most recent developments of electron diffraction methods. We participated in the organization of microsymposia at ECM30 in Basel and at XXIV IUCr Congress in Hyderabad India. We are especially interested in interdisciplinary microsymposia in order to disseminate knowledge of electron crystallography to other communities and also to a close collaboration with structural byologists and cryo EM scientists.

12. List SIG officers, name and e-mail, and specify their main function in the SIG: Mauro GEMMI, <u>Mauro.Gemmi@iit.it</u> chair Holger KLEIN, <u>holger.klein@grenoble.cnrs.fr</u> co-chair Lukas PALATINUS, <u>palat@fzu.cz</u> secretary Jérôme PACAUD, <u>jerome.pacaud@univ-poitiers.fr</u>, webmaster