ECA IET SIG No: 6

Reported Period: 2016-2017

Report Date: June 20th 2017

Reported by: Prof John R Helliwell DSc, IET Sig 6 Secretary on behalf of the Sig 6 Members

and the Sig 6 Chair Prof. Dr. h.c. Ullrich Pietsch

1. Introduction.

ECA IET Sig6 Chair *Ullrich Pietsch* and ECA IET Sig6 Secretary *John R Helliwell* have continued their roles. Their work has included submission of the suggestions from the SIG to the Programme Chair of ECM31 Oviedo.

2. SIG web site:

SIG 6's website is here:- http://ecanews.org/mwp/groups/sig-06-instrumentation-and-experimental-techniques/

The 2015 to 2016 report for example is here:

http://ecanews.org/mwp/wp-content/uploads/2016/08/SIG-6_-Annual-report_2016.pdf

3. Number of ECA individual members registered with the SIG

SIG 6 membership was 157 (checked on June 10th 2017).

4. Existence of a SIG mailing list?

Yes; the detailed instructions for using the email list can be found at the new ECA website and which are:-

Mailing List

Scientists which to participate to the SIG6 discussions should join the group's mailing list:

- mails can be sent to eca-sig6@listes.grenoble.cnrs.fr
- the archives can be consulted at https://listes.grenoble.cnrs.fr/sympa/arc/eca-sig6 (subscribers only, and you need to create an account by clicking on the "first login?" link at the top left)
- to **subscribe**, go to: https://listes.grenoble.cnrs.fr/sympa/subscribe/eca-sig6

• to **unsubscribe**, go to: https://listes.grenoble.cnrs.fr/sympa/sigrequest/eca-sig6

The mailing list engine is a SYMPA server, user information is available from: https://listes.grenoble.cnrs.fr/sympa/help/user

The list of commands you can send are listed in https://listes.grenoble.cnrs.fr/sympa/help/mail_commands (the list name is "era-sig6")

5. Approximate total number of researchers involved in the SIG (please indicate the basis for the estimate) 157 based on our registered list (checked on June 13th 2016).

6. List of MS proposed by the SIG for ECM31 Oviedo

Our Sig6 microsymposia proposals for the ECM31 Programme that we made early April 2017 are listed below:-

- 1. X-ray diffraction on the us to ps time scale
- 2. The use of ultra-hard x-rays for investigation of technical materials
- 3. New detectors for high energy x-ray applications (together with other SIGs)
- 4. The use of neutron scattering in nanoscience
- 5. Application of X-ray imaging techniques
- 6. Crystallisation for small and large molecules (together with other SIGs)

As Keynote speaker for the topic "Crystallization" we proposed Professor Naomi E. Chayen, Computational and Systems Medicine, Department of Surgery and Cancer, Faculty of Medicine.

7. Prizes awarded/sponsored/coordinated/received by Sig6 Members

At ECM30 Basle the Sig6 poster prize, winner details and our judging panel are summarised below:-

SIG 6 Jacek Grochowski	Anna Polyakova	MS3-P14: Tailor-made	Ulrich Pietsch (Chair)
Poster Prize	(EMBL-Hamburg)	beams for	Vincent Favre-Nicolin
100 Euro		macromolecular	John R Helliwell
		crystals on P14 at	
		PETRAIII	

8. Past Activities other than Microsymposia at ECM

8.1 John R Helliwell is Chair of the IUCr Diffraction Data Deposition Working Group, established at the Madrid IUCr Congress and confirmed to continue at the IUCr Montreal Congress by the IUCr Executive Committee. He Co-Organised the Research Data Management Workshop held at ACA 2017 in New Orleans, USA; for details, including presentations, see https://www.iucr.org/resources/data/dddwg/new-orleans-workshop

Naomi Chayen is a Management Committee Member of a European Commission COST Action on crystallization.

Naomi Chayen taught at the FEBS INSTRUCT Practical Crystallization Course. Novo Hrady, Czeck Republic.

Ullrich Pietsch is chair of the European Synchrotron User Organization (ESUO) representing about 30.000 European users of synchrotron sources and Free Electron Lasers. (http://www.wayforlight.eu/eng/esuo.aspx, www.ESUO.org).

Several SIG6 members gave invited and contributed talks on XTOP 2016, BRNO, http://xtop2016.sci.muni.cz/

8.X Summary of Outreach activities including contributions to the IYCr

As a contribution to this John R Helliwell published a new book entitled "Skills for a Scientific Life". The website is here:- https://www.crcpress.com/Skills-for-a-Scientific-Life/Helliwell/p/book/9781498768757. A Questions and Answers interview with the author can be found here:- https://www.crcpress.com/authors/i13576-john-r-helliwell/news/i3374-here-is-a-qanda-style-of-interview-of-me-by-crc-press

Realisation of the web site "Krystallopolis.com" http://www.krystallopolis.com/le-laboratoire/ which illustrates that Crystallography is the science that gives us clear views of the atomic and molecular structures inside matter - whether biological or mineral. It gives us, in other words, the keys we need to understand how the physical world works. Why, for example, can some materials conduct electricity whilst others provide good insulation? Why are some of them hard and others soft? How does an antibiotic work? etc. Crystallography provides the answers, by showing how materials are organised at the atomic level.

The 2017 HERCULES (Director: Vincent FAVRE-NICOLIN) course took place:-

Start Date 27th Feb 2017 End Date 30th Mar 2017

In addition to lectures and practicals in Grenoble (Institut Laue Langevin, ESRF and local laboratories), groups were also sent to Paris-Saclay (Soleil & the LLB, France), Hamburg (European XFEL and DESY, Germany), Villigen (Paul Scherrer Institute, Switzerland), and

Trieste (Elettra and the FERMI laser), i.e. including all European XFEL sites for the first time.

Naomi Chayen and her team ran a booth at the 2017 Imperial College Festival enabling members of the public to grow protein crystals and observe them under a microscope.

Naomi Chayen gave a DEB talk (similar to a TED talk) at the Royal Society London.

Naomi Chayen was interviewed by the National news agency of China - Xinhua News about crystallization of proteins.

Naomi Chayen was featured in 'Lab in the spotlight' in Crystallography Times speaking about a crystallization product that she has pioneered.

9. Future/Programmed Activities.

Sig 6 has put forward a wide range of microsymposia and keynote ideas for ECM31 in Oviedo. The Sig6 was represented at the ECM31 Programme Committee by the Sig 6 Chair Prof. Dr. Dr. h.c. Ullrich Pietsch.

10. Other contributions to crystallography

Entry of 'Microbatch' (the crystallisation method developed by Naomi Chayen and colleagues) in the Protein Data Bank search shows that the number of protein structures solved with crystals obtained using this technique continues to rise (e.g. **1,354** structures in 2016).

11. Other matters.

None to report.

12. Brief annual activity report

Our core function is to have assisted with the ECM next meeting program, ECM31.

We have been active in outreach.

The above details also show a real willingness to integrate and collaborate with IUCr on the matter of the availability of our raw diffraction data for all experimental methods of crystallography in addition to our processed diffraction data (such as structure factors or scattering curves/profiles) and our derived atomic and molecular data.

13. List SIG officers, name and e-mail, and specify their main function in the SIG:

Chair Prof. Dr. h.c. Ullrich Pietsch pietsch@physik.uni-siegen.de
Secretary Prof John R Helliwell DSc John.helliwell@manchester.ac.uk and Vice Chair Prof
Naomi Chayen n.chayen@imperial.ac.uk

Immediate past Chair Dr Thomas Tschentscher thomas.tschentscher@xfel.eu

Past Chairs: Dr Jean-Louis Hodeau jean-louis.hodeau@grenoble.cnrs.fr and Prof John R Helliwell DSc.

Members:-

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Supplementary Materials.

None.