

ECA IET SIG No: 6

Reported Period: 2015-2016

Report Date: July 17th 2016

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. Dr. h.c. Ullrich Pietsch

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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 ECM30 Basle.

The IET SIG6 Poster Prize is of course in memory of Professor Jacek Grochowski, Founding Vice Chairman of SIG6. The Judging Panel nominated for ECM30 comprises:- Chair: Prof Dr Ullrich Pietsch (SIG6 Chair, Germany) and Members; Prof John R Helliwell DSc (SIG6 Secretary and Poster Prize Sponsor, UK) and Dr Vincent Favre-Nicolin (SIG6 Webmaster, France). The presentation of the Prize at the ECM30 Closing Ceremony will be made by the Chair Prof Dr Ullrich Pietsch. The ECM 30 Poster Prizes Coordinator, Dr Bernhard Spingler [spingler@chem.uzh.ch], has been informed of our nominated Panel.

2. SIG web site:

SIG 6 url: <http://sig6.ecanews.org/> was updated with the 2014 to 2015 report.

3. Number of ECA individual members registered with the SIG

SIG 6 membership was 157 (checked on June 13th 2016).

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:-

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 ECM30 Basle

Our Sig6 microsymbosia proposals for the ECM30 Programme that we made on 1st May 2015 are listed below:-

1. X-ray diffraction on the μs 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)

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

John Helliwell received the 8th ECA Max Perutz Prize at the ECM29 in Rovinj.

At ECM29 Rovinj the Sig6 poster prize, winner details and our judging panel are summarised below:-



SIG 6 Jacek Grochowski Poster Prize Field: Instrumentation and Experimental Techniques Sponsor: SRS Daresbury Laboratory and the University of Manchester Prize: 100 euro	Ulrich Pietsch John R Helliwell Vincent Favre-Nicolin
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Marcin Stachowicz, *Biological and Chemical Research Centre, Chemistry Department, University of Warsaw, Poland*
[MS14-P5 Temperature and pressure induced phase transitions in chevkinite group. A joint XRD, XPS and EPMA structural studies]

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 ECM 29 Metadata for Raw Data Workshop held at ECM29 in Rovinj, Croatia; for an overview see <http://ecm29.ecanews.org/metadata/> and program details see <http://www.iucr.org/resources/data/dddwg/rovinj-workshop>

Naomi Chayen is a member of a Review Panel selecting projects using the Brookhaven National Laboratory Synchrotron Source, USA (current).

Ulrich 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).

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

As a contribution to this John R Helliwell published a new book entitled “*Perspectives in Crystallography*” (CRC Press, November 2015). It includes sections such as ‘*Explaining “What is crystal structure analysis?” for general audiences*’; ‘*Celebrating the Centennial of X-ray crystal structure analysis*’; ‘*Aspects of crystallography research*’; ‘*The societal impacts: Crystal structure analysis and the sustainability of Life*’. This is a contribution to continuing the IYCr’s legacy.

John Helliwell presented a talk (<http://www.iucr.org/education/presentations/crystallography-and-sustainability>) in the American Crystallographic Association Transactions Symposium on Crystallography and Sustainability in Philadelphia, USA July 2015. John Helliwell’s

article and indeed the whole Symposium proceedings volume can be found here:-
<http://www.amercrystalassn.org/documents/2015%20Transactions/volume45.pdf>

Naomi Chayen and her team set up a stand entitled '*Crystals – Beauty and Utility*' at the Imperial Festival 2016.

Lata Govada from Naomi Chayen's team gave a TEDx Brixton talk (October 2015).

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 2016 HERCULES (director: Vincent FAVRE-NICOLIN) course took place from 29 March to 29 of April. It welcomed 79 participants of 26 different nationalities and who are working in 23 different countries. Participants were selected from a record number of applicants (>160). 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.

9. Future/Programmed Activities.

Sig 6 has put forward a wide range of microsymbosia and keynote ideas for ECM30 in Basle. The Sig6 was represented at the ECM30 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 (currently at **1,354** structures).

11. Other matters.

None to report.

12. Brief annual activity report

Our core function is to have assisted with the ECM next meeting program, ECM30.

We have been active in outreach, including assisting with the IYCr legacy moving forward.

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. 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:-

sgg@uniovi.es

m.lutz@uu.nl

tilo.baumbach@kit.edu

heger@xtal.rwth-aachen.de

heribert.wilhelm@diamond.ac.uk jordi.juanhuix@cells.es

e.saridakis@imperial.ac.uk

i.robinson@ucl.ac.uk

b.cernik@manchester.ac.uk

vincent.favre-nicolin@cea.fr

jrc@ill.fr

rene.guinebretiere@unilim.fr

Supplementary Materials.

None.