

ECA IET SIG No: 6

Reported Period: 2014-2015

Report Date: July 14th 2015

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

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 Judging Panel for ECM29 is now confirmed in good time before ECM29; this Prize is of course in memory of Professor Jacek Grochowski, Founding Vice Chairman of SIG6. The Panel comprises:- Chair: Prof Dr Ulrich 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 ECM29 Closing Ceremony will be made by the Chair Prof Dr Ulrich Pietsch. The ECM 29 Poster Prizes Coordinator, Dr Biserka Prugovečki, has been informed.

2. SIG web site:

SIG 6 url: <http://sig6.ecanews.org/> was updated with the 2013 to 2014 report.

The Secretary regrets that the annual reports of the first few years of the SIG6 cannot at present be located; the search for these continues! They will of course be in the ECA formal archives of the ECA Executive Committee (printed) minutes (held in the Netherlands) but not thereby at the Sig6 website, where a copy would be beneficial.

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

SIG 6 Instrumentation and experimental techniques was 162 for 2013 to 2014 and has now increased to 210 for the year 2014 to 2015 (checked on June 30th 2015).

4. Existence of a SIG mailing list?

Yes

Address of the mailing list: eca-sig6@listes.grenoble.cnrs.fr

Number of members in the SIG mailing list : 15

5. Approximate total number of researchers involved in the SIG (please indicate the basis for the estimate) 210 based on our registered list (checked on June 30th 2015). [We realise this is the same answer as we gave to question 3, and indeed the activity is probably more, but we would appreciate guidance from the ECA Executive Committee as to what other estimate might be made?]

6. List of MS organized by the SIG at the last ECM 28 Warwick

[We apologise but have misplaced the finalised, full, list.]

We are happy to mention though:-

Ullrich Pietsch chaired MS 22 at the ECM in Warwick on, *Materials studied by coherent diffraction imaging* with 6 speakers and about 50 participants.

John R Helliwell presented the IET Sig 6 Jacek Grochowski poster prize to Dr Semen Gorfman at the ECM 28 Closing Ceremony. JRH chaired a MS on *XFEL and time-resolved crystallographic methods*.

We appointed Ullrich Pietsch to represent SIG-6 at the ECM-29 Croatia program committee. Nb 2014 was the IUCr Congress Year ie no ECM.

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

It was announced that John R Helliwell is to be the recipient of the ECA 8th Perutz Award at the ECA ECM29 2015 to be held in August in Rovinj, Croatia.

Sahir Khurshid, Lata Govada and Naomi Chayen won the 3rd Prize in the category of Innovation of the EPSRC Science Photography competition (March 2015)

<https://www.flickr.com/photos/epsrc/15976067595/in/set-72157651335202305>

8. Past Activities other than Microsymposia at ECM

8.1 *Naomi Chayen* has been selected as a management committee member on a European Commission - European Cooperation in Science & Technology (COST), A new collaborative initiative entitled 'From molecules to crystals' involving over 30 groups across Europe (Nov 2014-2018).

A paper by the Chayen team about designing the first nucleation inducing agents for automated crystallization trials so that they can be used for high throughput published in March 2015 in *Acta Crystallographica D* 71, 534-540 got highlighted as Research News by the **International Union of Crystallography** and other websites.

A commercial product based on the research called '*Chayen Reddy MIP*' has been launched by Imperial Innovations. <http://www.imperialinnovations.co.uk/CRMIP>

Naomi Chayen and Lata Govada lectured and demonstrated at the FEBS-INSTRUCT crystallisation course in the Czech Republic entitled 'Advanced methods in macromolecular crystallization' (June 2014).

8.2 *Vincent Favre-Nicolin* was Chair of the XTOP2014 conference <http://xtop2014.org/>, which took place in Grenoble & Villard-de-Lans (F), in September 14-19th 2014; he was Chair of the HERCULES Courses in Grenoble (F) held *March 1st to April 1st, 2014. and March 2nd to April 1st, 2015.*

8.3 *Hervé Guinebretière* was chair of the AICr2014 committee in France and is President of the French Association of Crystallography and was the co-chair of the scientific committee of the AFC-Conference in Bordeaux (F) *July 02-05 2014* and is co-chair of the RX & Matière conference in Grenoble (F) 01-04 dec. 2015, <http://www.rayonsxetmatiere.org/>

8.4 *Jean Louis Hodeau* is a member of the AICr2014 committee in France, he was chair of the committee which built multilingual hands-on travelling exhibitions "*A journey into the crystal*" and is co-chair of the RX & Matière conference which will take place in Grenoble (F) 01-04 dec. 2015, <http://www.rayonsxetmatiere.org/>

8.5 *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 has Co-Organised the ECM 29 Metadata for Raw Data Workshop to be 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>

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

Naomi Chayen, Lata Govada and Elspeth Garman gave an outreach lecture with live demonstrations of crystals growing under a microscope at a conference for 140 executives from companies and organisations (e.g. Expedia, BT, Ministry of Defence). The conference was called ITT Vanguard - European Next (and was held in the summer 2014).

Naomi Chayen and her team set up a stand entitled 'Making Complexity Crystal Clear' at the Imperial Festival 2015 where they highlighted the importance of protein crystals and their role in the facilitation of drug design.

Naomi Chayen and Lata Govada Exhibited at the British Crystallography Association in UK's biggest Science and Engineering event, the Big Bang Science Fair (held March 2015) Lata Govada spoke at the Soapbox Science event organised by L'Oreal and sponsored by STFC Research Council (held June 2015)

John R Helliwell presented a lecture at Strathclyde University entitled "A century of X-ray crystal structures: from common salt to enzymes in high salt" (December 2014).

9. Future/Programmed Activities.

SIG 6 has put forward a wide range of microsymbosia and keynote ideas for ECM30 in Basle. The SIG6 is represented by the SIG 6 Chair Prof. Dr. Dr. h.c. Ullrich Pietsch.

As a contribution to assisting the momentum of the IYCr into the future John R Helliwell has prepared a new book entitled "Perspectives in Crystallography" to be published by CRC Press in 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'.

10. Other matters.

None to report.

11. Brief annual activity report

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

We have also been active in outreach, including various IYCr activities and have plans to assist 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 in addition to our processed structure factors and our derived molecular data.

12. 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.*

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Supplementary Materials.

None