

ECA IET SIG No: 6

Reported Period: 2018-2019

Report Date: July 17th 2019

Reported by: Dr. Michele Cianci, 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* continued its role. ECA IET Sig6 Secretary position was left vacant from *John R Helliwell* and passed over to *Michele Cianci* after the ECM31 Oviedo. For the first half of 2018 *Ullrich Pietsch's* and *John R Helliwell's* work has included submission of the suggestions from the SIG to the Programme Chair of ECM31 Oviedo. Also two workshops have been organised at ECM31, one with the Chairman and the (<http://ecm31.ecanews.org/en/progress-instrumentation-x-ray-diffraction-and-cryoem.php>) and one with the Secretary (<http://ecm31.ecanews.org/en/neutron-macromolecular-crystallography.php>).

2. SIG web site:

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

The 2017 to 2018 report for example is here:

https://ecanews.org/wp-content/uploads/2018/08/SIG6_Annual-report_2017-2018.pdf

3. Number of ECA individual members registered with the SIG

SIG 6 membership was 95 (checked on July 16th 2019).

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) 95 based on our registered list (checked on July 16th 2019).

6. List of MS proposed by the SIG for ECM32 Wien

Our Sig6 microsymbosia proposals for the ECM32 Programme that we made in May 2018 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
4. The use of x-rays and neutrons for experiments in nanoscience
5. Application of X-ray imaging techniques
6. Crystallisation for small and large molecules
7. Robotics and its software for crystallization
8. Long wavelengths instrumentation and methods

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

At ECM31 Oviedo the Sig6 poster **prize, winner details and** our judging panel are summarised below:-

SIG 6 Jacek Grochowski Poster Prize, 100 Euro	
Judging Panel	Ulrich Pietsch (Chair), Krzysztof Wozniak, Michele Cianci
Researcher	Shoichi Uechi (Ibaraki University, Tokai, Japan)
MS and Poster	MS39-P03

Title	Local structure observation of Sm doped RB6 (R: rare earth) by white neutron atomic resolution holography
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8. Past Activities other than Microsymposia at ECM

8.1 Workshops

The details of two Workshops at ECM31 Oviedo organized by the Sig6 members are summarized as follow:

Title	Progress in instrumentation for X-ray diffraction and CryoEM
Organisers:	Prof. Dr hab. Krzysztof Woźniak (University of Warsaw, Poland), Chair Prof. Dr. Ullrich Pietsch, (Universität Siegen, Germany), Co-chair. Dr Michele Cianci (Università Politecnica delle Marche, Italy), Co-chair.
Jointly with	SIG2
When	22 August, 2018, from 9:00 to 17:30.
Participation fee	60 euro
Speakers	13
Attendees	50
Website	https://ecm31.ecanews.org/en/progress-instrumentation-x-ray-diffraction-and-cryoem.php
Abstract booklet	https://ecm31.ecanews.org/archivos/pdf/Satellite_Abstacts_all_Final.pdf
Short description	This satellite meeting presented an overview of a wide range of new laboratory instrumentation available from different companies, as well as new developments at several large scale facilities. The meeting covered information on the newest laboratory instruments from Bruker and Rigaku as well as on new instrumental solutions such as the Lyncean Compact Light Source (CLS) and Sigrey's newest X-ray sources and optics, and focus on bringing world-class structural and analytical synchrotron type capabilities back to our labs. We organised sessions focused on new photon sources to be installed at major European synchrotrons as well as X-ray Free Electron Laser facilities including ESRF, DESY, MAXIV, and the Swiss and European X-FELs. The organisers are also particularly proud to advertise some of the first experimental results taken at European X-FEL. The program of this satellite was complemented by news from the neutron ISIS facility and from the cryo-EM equipment producers to provide a forum to discuss the future of instrumentation for X-ray, neutron diffraction and CryoEM.

Title	Neutron macromolecular crystallography for structural chemistry and biology studies that are at an impasse with other techniques
Organisers:	John R Helliwell (University of Manchester), Chair. Matthew Blakeley & Nicholas Coquelle (Institut Laue-Langevin), Co-Chairs.

	Zoe Fisher (ESS, Lund). Tobias Schrader (JCNS, Julich).
Jointly with	n/a
When	21 August 2018, from 14:00 to 19:00; 22 August 2018, from 9:00 to 17:00.
Partecipation fee	60 euro
Speakers	18
Attendees	20
Website	https://ecm31.ecanews.org/en/neutron-macromolecular-crystallography.php
Short description	<p>This Workshop highlighted recent studies which exemplify how nMX moves forward structural chemistry and biology studies of protein function that were otherwise at an impasse with other probes of matter. Also we highlighted new instrumentation and software developments.</p> <p>The report on this Workshop is available in the IUCr Newsletter at:- https://www.iucr.org/news/newsletter/volume-27/number-1/neutron-macromolecular-crystallography-workshop-at-ecm31</p>

Title	XTOP 2018. XIV Biennial Conference of High Resolution X-ray Diffraction and Imaging
Organisers:	http://www.ba.ic.cnr.it/xtop2018/
Jointly with	n/a
When	From 03/09/2018, 9am to 07/09/2018, 4pm
Partecipation fee	n/a
Speakers	18
Attendees	20
Website	http://www.ba.ic.cnr.it/xtop2018/
Short description	XTOP brings together scientists from the fields of X-ray diffractometry, reflectometry, standing waves, coherent and conventional X-ray diffraction imaging and topography, as well as X-ray absorption and phase contrast imaging. XTOP is thus one of the central scientific conference concerning methods and instrumentation in laboratory and synchrotron-based high-resolution X-ray diffraction methods, phase contrast imaging, and micro-tomography.

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

·Structural Biology Theme lead at Imperial for the Rosalind Franklin Institute

- Featured in Chemistry World News: “The Protein Crystallisation Influencer” (March 2019)
- Plenary speaker at MIPs international conference “MIPs for Crystals” (June 2018)
- Chair of the Crystallization session at the 2018 BCA Meeting
- Programme Committee Member for the International Conference for Crystallization of Biological Macromolecules (ICCBM) Shanghai (Nov 2018).
- Speaker at FEBS INSTRUCT Practical Crystallization Course. Novo Hrad, Czech Republic (June 2018)
- Speaker at EMBO High Throughput Protein Production and Crystallization Course. Harwell (June 2019)
- Keynote Lecture at ECM32 “Enhancing the Success of Macromolecular Crystallization”

8.3 John Helliwell, Founding Chairman and a Past Secretary of ECA IET Sig6, is Lead Organiser of “Data Science Skills in Publishing” Satellite Workshop at ECM32 Vienna sponsored by IUCr. Details are here :- <https://www.iucr.org/resources/data/commdat/vienna-workshop>

8.4 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).

10. Summary of Outreach activities

10.1 Naomi Chayen

- Exhibitor at the Imperial Festival 2018
- Exhibitor at the Great Exhibition Road Festival 2019

The stands in both Festivals highlighted the importance of protein crystals and crystallography in facilitating drug design.

10.2 Vincent FAVRE-NICOLIN

The 2019 HERCULES (Director: Vincent FAVRE-NICOLIN) details are here:- <http://hercules-school.eu/55-organizing-committee.htm> 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.

11. Future/Programmed Activities.

Sig 6 is assembling microsymbiosia and keynote ideas for ECM33 in Prague. Sig6 will be represented at the ECM33 Programme Committee by the Sig 6 Chair Prof. Dr. Dr. h.c. Ullrich Pietsch.

12. Other contributions to crystallography

John R Helliwell is a Programme Committee Member for the World Congress of Crystallography to be held in Prague in 2020. He is also the IUCr Representative to the International Council of Science Committee on Data ('CODATA'). He is Chair of the **IUCr/Oxford University Press (OUP) Book Series Selection Committee**, details of which can be found here:- <https://www.iucr.org/iucr/governance/advisory-committees/book-series> .

13. Other matters.

None to report.

14. Brief annual activity report

Our core function is to have assisted with the ECM next meeting program, ECM33.

We have been active in outreach.

The above details also show a real willingness to integrate and collaborate with IUCr on the matters of policy re crystallographic data and which includes:- encouraging 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.

John R Helliwell has continued his outreach books within which crystallography examples feature. In this last year he has published: *The Whys of the Scientific Life*, details of which are here:- <https://www.crcpress.com/The-Whys-of-a-Scientific-Life/Helliwell/p/book/9781138389793>

15. 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 Dr. Michele Cianci m.cianci@univpm.it 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.*

Immediate past secretary Prof. John R. Helliwell John.helliwell@manchester.ac.uk

Members:-

Other members:

- Tilo Baumbach (D)
- Robert Cernik (UK)
- Naomi Chayen (UK)
- Vincent Favre-Nicolin (F) – webmaster
- Santiago Garcia Granda (SP)
- Heger Gernot (G)
- René Guinebretière (F)
- John R. Helliwell (UK)
- Jean-Louis Hodeau (F)
- Jordi Juanhuix (S)
- Martin Lutz (NL)
- Ake Kvik (S)
- Ian Robinson (UK)
- Juan Rodriguez-Carvajal (F)
- Emmanuel Saridakis (GR)
- Thomas Tschentscher (G)
- Heribert Wilhelm (UK)

Supplementary Materials.

None.