

ECA IET SIG No: 6

Reported Period: 01/2021 - now

Report Date: July 18<sup>th</sup> 2022

Reported by: Prof. 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 *Michele Cianci* continued its role.

For 2019-21 *Ullrich Pietsch*'s and *Michele Cianci*'s work has included submission of the suggestions from the SIG to the Programme Chair of ECM33 Versailles.

The Secretary chaired one session (MS-31: Recent advances in instrumentation). at IUCR25 (Prague). Details are available at:  
([https://www.conftool.com/iucr2020/index.php?page=browseSessions&form\\_session=189](https://www.conftool.com/iucr2020/index.php?page=browseSessions&form_session=189))

## **2. SIG web site:**

SIG 6's website is here:-

<https://ecanews.org/groups/sig-06-instrumentation-and-experimental-techniques/>

The 2018 to 2019 report for example can be found here:

[https://ecanews.org/wp-content/uploads/2019/08/Report-SIG6\\_2019.pdf](https://ecanews.org/wp-content/uploads/2019/08/Report-SIG6_2019.pdf)

The report covering the 2019-20 period was submitted on the 8<sup>th</sup> of February 2021, but it has not been uploaded.

## **3. Number of ECA individual members registered with the SIG**

SIG 6 membership was 61 (checked on July 18<sup>th</sup> 2022).

## **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](mailto: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](https://listes.grenoble.cnrs.fr/sympa/help/mail_commands) (the list name is “era-sig6”)

## **6. List of MS proposed by the SIG for ECM33 Versailles**

Our Sig6 microsymbiosia proposals for the ECM33 Programme that we made in December 2019 are listed below:-

1. X-ray diffraction on the  $\mu\text{s}$  to ps time scale (as in ECM31)
2. The use of nanobeams for investigation of technical materials
3. New detectors for FEL applications (together with other SIGs)
4. Artificial intelligence in Photon and neutron crystallography (NEW)
- 5 The use of x-rays and neutrons for experiments in nanoscience (as in ECM32)
6. Application of X-ray imaging techniques
7. Crystallization for small and large molecules (together with other SIGs)

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

At ECM32 Vienna the SIG6 poster **prize, winner details and** our judging panel are summarised below:-

SIG 6 Jacek Grochowski Poster Prize, 100 Euro
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Judging Panel	Michele Cianci (Chair), Thompson Andrew, Annalisa Guerri
Researcher	Ceretti Monica, CNRS Montpellier (France)
MS and Poster	MS42-P01
Title	" Phase Diagram and Redox Behavior of (Nd/Pr) <sub>2</sub> NiO <sub>4+d</sub> Electrodes Explored by in situ Neutron Powder Diffraction

## 8. Past Activities other than Microsymposia at ECM

### 8.1 Schools

The details of AICS2021 International School of Crystallography organized by the Sig6 members are summarized as follow:

Title	Fundamentals of Crystallography: the theory behind crystal structure solution
Organisers:	Chair Dr. Paolo Mazzeo (University of Parma, Italy), Prof. Elisa Boanini, (University of Bologna, Italy), Prof. Michele Cianci (Università Politecnica delle Marche, Italy), Dr. Danilo Belviso (CNR – Bari).
Jointly with	none
When	from the 31st of August till the 4th of September 2021
Partecipation fee	60 euro
Speakers	13
Attendees	50
Website	<a href="https://cristallografia.org/aicschool2021/eng/detail.asp?idn=4401">https://cristallografia.org/aicschool2021/eng/detail.asp?idn=4401</a>
Short description	the AICS2021 school was about fundamentals of crystallography, and it is thought for students and researchers wishing to exploit crystallographic techniques in their research for the first time or those who already use crystallography and want to deepen basic theoretical aspects. Chemists, biologists, and physicists are the main recipients of the school. To level participants' knowledge out, a pre-course of half day for essential math and physics will be held.

### 8.2 Workshops

Title	MS-31: Recent advances in instrumentation at IUCR25 Prague
Organisers :	Chair Prof. Michele Cianci (Università Politecnica delle Marche, Italy), and Co-Chair Prof. Zschech, Ehrenfried (Fraunhofer-Institut für Keramische Technologien und Systeme IKTS)
Jointly with	none
When	Monday, 16/Aug/2021: 2:45pm - 5:10pm
Partecipati on fee	n/a

Speakers	6
Attendees	18
Website	<a href="https://www.conftool.com/iucr2020/index.php?page=browseSessions&amp;form_session=189">https://www.conftool.com/iucr2020/index.php?page=browseSessions&amp;form_session=189</a>
Short description	<p>This symposium focused on new Instruments and Experimental Techniques related to synchrotron-radiation, FEL, neutrons and combined methods. The symposium offers the opportunity for scientists to showcase their facilities with the aim of promoting access and awareness among a wide, non-specialist audience.</p> <p>The symposium will feature invited talks from Dr. Wenbing Yun (Sigray, Inc., USA) and Dr. Andrew Thomson (SOLEIL Synchrotron, France).</p>

John R Helliwell was a Programme Committee Member for the World Congress of Crystallography to be held in Prague in 2021. He is also the IUCr Representative to the International Council of Science Committee on Data ('CODATA'). He was 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> .

**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** John Helliwell has worked as Scientific Chairman of the AICS2021 school. The lecturer line-up included:

Massimo Nespolo, Université de Lorraine, FR

Gervais Chapuis, École Polytechnique Fédérale de Lausanne, CH

Lukas Palatinus, Institute of Physics of the Czech Academy of Sciences, CZ

Regine Herbst-Irmer, University of Gottingen, D

Isabel Uson, Institute de Biologia Molecular de Barcelona, SP

The school was held online on THOLA virtual event platform.

## 10. Summary of Outreach activities

One Crystallographic School and one microsymbosia at IUCR25 were organized. Several other committees on crystallographic related matters were chaired.

## 11. Future/Programmed Activities.

Sig 6 is assembling microsymbosia and keynote ideas for ECM34 in Padova (IT). Sig6 will be represented at the ECM34 Programme Committee by the newly appointed Sig 6 Chair.

Prof. Dr. Dr. h.c. Ullrich Pietsch has announced his retirement as Chair of Sig-06. The ECM33 Sig-06 meeting will discuss proposals and elect his successor.

## **12. Other contributions to crystallography**

n/a

## **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.

Overall Sig6 shows 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.

Michele Cianci, as member of the AIC Commission for Crystallography Teaching and the Scientific Committee of the School, is actively engaged in organizing the yearly schools of the Italian Crystallographic Association.

## **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 Prof. Michele Cianci* m.cianci@univpm.it

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

*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 Kvick (S)
- Ian Robinson (UK)
- Juan Rodriguez-Carvajal (F)
- Emmanuel Saridakis (GR)
- Thomas Tschentscher (G)
- Heribert Wilhelm (UK)

**Supplementary Materials.**

None.