ECA IET SIG No: 6

Reported Period: 2019-20120

Report Date: February 8th 2020

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 SIG-6 Chair *Ullrich Pietsch (UP)* and ECA IET SIG-6 Secretary *Michele Cianci (MC)* continued their role. For the first half of 2019 *Ullrich Pietsch's* and *Michele Cianci's* work has included the preparation of ECM32 Wien. Also, one workshop and one microsymposia have been organised at ECM32, one by John Helliwell and one by Naomi Chayen (see details below). In the first half of 2020 a list of possible MS for ECM33 was defined by UP and MC. MC worked on the preparation of the microsymposium 246 "Recent advances in instumentation" at IUCr 2020.

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

3. Number of ECA individual members registered with the SIG

SIG 6 membership was 98 (checked on February 1st 2021).

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) 98 based on our registered list (checked on February 1st 2021).

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

1. X-ray diffraction on the μs 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)

Key note in the field of "Crystallography in Nanoscience" is Anna Foncuberta I Morral (EPF Lausanne) (not confirmed)

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

At ECM32 Wien the Sig6 poster **prize, winner details and** our judging panel are summarised below:-

SIG 6 Jacek Grochowski Poster Prize, 100 euro + 150 euro from the Organizing Committee

Judging Panel	Ulrich Pietsch (Chair), Annalisa Guerri, Andrew Thompson
Researcher	Ceretti Monica
Presentation photo	
MS and Poster	MS42-P01
Title	Phase Diagram and Redox Behaviour of (Nd/Pr)2NiO4 Electrodes Explored by in situ Neutron Powder Diffraction

8. Past Activities other than Microsymposia at ECM

8.1 Workshops

The details of two Workshops at ECM32 Wien organized by the Sig6 members are summarized as follow:

Title	"Data Science Skills in Publishing" Satellite Workshop
Organisers:	John Helliwell (University of Manchester, UK), Brian McMahon (IUCr, R&D Department, UK)
Jointly with	n/a
When	18th August 2019 (1 day), Time: 8:25 a.m. to 5 p.m
Partecipation fee	n/a
Speakers	12
Attendees	23
Website	https://www.iucr.org/resources/data/commdat/vienna-workshop
Abstract booklet	https://www.iucr.org/__data/assets/pdf_file/0014/144005/programme.pdf
Short description	There is a trend towards ensuring that modern science research data are findable, accessible, interoperable and reusable (FAIR). However, this is something that crystallographers have been achieving for many decades, during which excellent crystallographic databases have always exploited the best available hardware for digital archiving. FAIR is necessary but not sufficient, as physicists would say, as the archived data should also

	be true facts. So FACT and FAIR are needed for reproducibility. The crystallographic community has developed automatic checking software by pooling its experiences from hundreds of thousands of crystal structure analyses into validation procedures with numerous data file checks on both coordinates and processed diffraction data sets. Alarm alerts can then be scrutinised by journal editors and referees. With such exemplary procedures is there anything to be improved? Crystallographers conclude that there is. Firstly the IUCr journal *Acta Cryst. C: Structural Chemistry* has always required submission of article with validation report with underpinning data files. Thus the specialist subject expertise of referees can involve their own direct calculations to supplement the automatic checks before article and data set acceptance as versions of record by the editor. This has inspired others to look to improve their own crystallographic disciplines and journals to follow the *Acta Cryst. C* standard. Secondly the digital archives have enhanced their capacity in recent years owing to amazing hardware advances so that even the Gigabyte-sized raw data sets can also be preserved as versions of record. A reader of a publication can thereby revisit even the earliest calculation decisions of the authors of a publication. As the Royal Society of London puts it: science is about not taking someone's word and so, instead, the science is always in the data. FACT and FAIR, indeed scientific objectivity itself, is possible. This Workshop will address the state of the art in the field and the data science skills hoped for, indeed to be expected, of all those involved in publishing crystallography results, and of results from all the cognate methods such as scattering, microscopy and spectroscopy.

Title	Micro symposia on Crystallization of small and large molecules
Organisers:	Naomi E. Chayen (Imperial College London, United Kingdom), May Marsh Sharpe (Paul Scherrer Institut, Switzerland)
Jointly with	n/a
When	Date: Tuesday, 20. August 2019, Time: 14:00 - 16:00
Partecipation fee	n/a
Speakers	5
Attendees	n/a
Website	https://www.ecm2019.org/programme/microsymposia/focus-area-5-experimental-and-computational-techniques/ms41-crystallisation-of-small-and-large-molecules/
Abstract booklet	https://www.ecm2019.org/fileadmin/user_upload/k_ecm2019/images/Programm/ECM32AbstractBooklet_18.08.2019.pdf, Page 648
Short description	The focus of microsymposia was on strategies, techniques and tools for obtaining useful crystals of small and of large molecules for x-ray crystallography.

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

8.3 John R Helliwell is a Programme Committee Member for the World Congress of Crystallography to be held in Prague in 2021 as representative of the IUCr Committee on Data. He is also the IUCr Representative to the International Council of Science Committee on Data ('CODATA') and Chair of the IUCr's Committee on Data. He is Chair of the IUCr/Oxford University Press (OUP) Book Series Selection Committee. He chaired the Search and Interviews Committee for the next Editor-in-Chief of the journal Structural Dynamics published by the American Institute of Physics and the American Crystallographic Association. He is now an Editorial Advisory Board Member for Crystallography Reviews. He is a Guest Editor for IUCr Journals' Acta Cryst D for the International Symposium on Diffraction Structural Biology 'ISDSB2019' Collection of Articles.

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).

8.5 Michele Cianci is member of the Italian Delegation to the European Synchrotron User Organization (ESUO). He is also member of the Teaching Commission for the Italian Association of Crystallography (AIC).

10. Summary of Outreach activities

10.1 Naomi Chayen

- Keynote lecture at the European Crystallography Meeting. Vienna, Austria (August 2019)
- Chair of Micro symposia on Crystallization of small and large molecules. European Crystallography Meeting Vienna, Austria (August 2019)
- An interview with Nature (still face to face) for a Nature podcast about crystallization of proteins in March 2020.
- Crystallisation workshop (face to face) at Imperial College (January 2020)

10.2 John Helliwell

- John R Helliwell has continued his outreach books within which crystallography examples feature. In October 2019 he has published The Whats of a Scientific Life https://www.routledge.com/The-Whats-of-a-Scientific-Life/Helliwell/p/book/9780367233020.

10.3 Michele Cianci

- Speaker at ESRF (Grenoble, (FR)), User meeting 2020, MicroSymposium on Multi-crystal and serial data collection in Structural Biology. "Theory and Methods in Microcrystallography of Biological Macromolecules".

- Together with Prof. Zschech, Ehrenfried (Fraunhofer-Institut für Keramische Technologien und Systeme IKTS) MC will be co-chair of the microsymposium 246 “Recent advances in instumentation“ at IUCr 2020 (see http://www.xray.cz/iucr/tmp/chairs.asp?id=246).

10.4 Ullrich Pietsch

Member of the German delegation of SIG-6 members to the Joint Polish-German Crystallographic Meeting 2020 held on the 24-27 February in Wroclaw, Poland.

11. Future/Programmed Activities.

SIG-6 is assembling microsymposia and keynote ideas for ECM33 in Versailles. SIG-6 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

Most if not all our activities have been hampered by the continuing pandemic situation.

Our core function is to assist 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

Vice Chair Prof Naomi Chayen n.chayen@imperial.ac.uk
Secretary Prof. Michele Cianci m.cianci@univpm.it

and

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

Supplementary Materials.

None.