SIG4 activity report September 2022-September 2023

- Editorial activity of SIG members

Joke Hadermann: co-editor of Acta Cryst B (IUCr), Journal of Solid State Chemistry (Elsevier), Batteries (MDPI)

Lukas Palatinus: co-editor of Acta Cryst A (IUCr)

Tatiana Gorelik: co-editor of Acta Cryst A (IUCr)

Xiaodong Zou: main editor, section for Electron crystallography, IUCrJ

Mauro Gemmi, co-editor, section for Electron crystallography, IUCrJ

Louisa Meshi, co-editor, section for Electron crystallography, IUCrJ

Tatiana Latychevskaia, editor at Scientific Reports

Enrico Mugnaioli, Stavros Nicolopoulos, Partha Pratim Das: guest editors - special issue- Symmetry (MDPI)

Damien Jacob, co-editor in chief of the The European Physical Journal Applied Physics (EPJAP)

- Organization of ECM

SIG4 representative in the organizing committee of ECM33 in Versailles 2022 – Andy Stewart

List of MSs @ECM33 organized by SIG:

MS24 3D electron diffraction

MS25 3D electron diffraction for structure solution of organics and proteins

MS39 Crystallography at the nanoscale

MS13 Structural Characterization of Functional Materials

MS17 Total scattering studies and disorder

MS28 Navigating crystal forms in molecular and pharmaceutical materials

MS30 Advanced porous materials: MOFs, COFs, SOFs....and what else?

MS37 Advances in Structure determination of new materials by multi-technique approach including imaging techniques

MS43 Crystallography for cultural heritage materials

SIG4 representative in the organizing committee of ECM34 in Padova 2024 – Anton Cleverley

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- SIG4 webpage and mail list

Webpage is on and frequently updated. Webpage administrator Tim Gruene.

https://ecaelectronsig.wordpress.com/

Mail list administrator is Jérôme Pacaud jerome.pacaud@univ-poitiers.fr

The mail list contains 114 members. During the last year the mail list was used for 4 webinar and online lecture announcements; 4 workshop, conference and school announcements, 5 position offerings, 1 workshop report. The other messages in the mail list are related to the SIG4administration.

- Prizes sponsored/coordinated

Poster prizes @ECM33

ELDICO SCIENTIFIC sponsored poster prize: Barbara Gruza, "TAAM refinement in dynamical approach against electron diffraction data"

NANOMEGAS sponsored two poster prizes:

Sara Passuti, "3D scanning precession electron diffraction analysis of nanodomains in thin films" and Laura Gemmrich Hernández "Structure solution using 3DED of beam and vacuum sensitive carbazole-based di-phosphonic acid Metal Organic Frameworks"

SIG4 distinguished publication award:

2023: Meng Ge, Taimin Yang, Hongyi Xu, Xiaodong Zou, and Zhehao Huang: "Direct Location of Organic Molecules in Framework Materials by Three-Dimensional Electron Diffraction." JACS (2023) 144, 15165−15174, DOI: 10.1021/jacs.2c05122

https://www.iucr.org/news/newsletter/etc/articles?issue=156393&result_138339_result_page=32

Organization of dedicated schools / workshops

- Electron Crystallography School, 29 August – 1 September 2022, Satellite to ECM33, Caen, France

Number of Participants: 47

Level of involvement of SIG in the activity: organization, lecturing

ECA Individual Members registered with the SIG involved in the organizing committee: yes

ECA Individual Members registered with the SIG involved as lecturers: yes

SIG endorsed (SIG logo on the web page/leaflets): yes

Sponsored by ECA (Yes/ No)? no

Short Description: The school will cover diverse theoretical and practical aspects of 3D electron diffraction technique (3D ED / microED) and its application to structure determination of nano/microcrystalline materials of different classes – from inorganic, to organic and biological compounds. The school will include lectures and tutorials demonstrating the use of electron diffraction

data for structure analysis. We plan a poster session, where students can present their work and a panel discussion about the future developments of 3D ED.

Web address: https://school2023.cristallografia.org/

- Workshop "electron diffraction for structural crystallography", Aussois, France, 17-21 October 2022

Number of Participants: 48

Level of involvement of SIG in the activity: organization, and lecturing by several SIG Members

ECA Individual Members registered with the SIG involved in the organizing committee: yes (Philippe Boullay, Stéphanie Kodjikian)

ECA Individual Members registered with the SIG involved as lecturers: yes (Lukas Palatinus, Philippe Boullay, Stéphanie Kodjikian)

SIG endorsed (SIG logo on the web page/leaflets): no

Sponsored by ECA (Yes/ No)? no, not applied for

Short description: Workshop on 3D-ED for X-ray crystallographers in materials sciences and life sciences. Program (lectures and tutorials): basics of transmission electron microscopy, 3D ED data acquisition techniques, structure solution, dynamical refinement.

Web address: https://cdifx.univ-rennes1.fr/RECIPROCS/ANF2022/ANF2022_Aussois.htm

- Introduction to Three-Dimensional Electron Diffraction / MicroED, 28 January 2023, 27th Australian Conference on Microscopy and Microanalysis, Australia

Number of Participants: 10

Level of involvement of SIG in the activity: organization, lecturing

ECA Individual Members registered with the SIG involved in the organizing committee: yes

ECA Individual Members registered with the SIG involved as lecturers: yes

SIG endorsed (SIG logo on the web page/leaflets): yes

Sponsored by ECA (Yes/ No)? no

Short Description: The workshop covered basic theoretical and practical aspects of 3D electron diffraction technique (3D-ED / microED) and its application to structure determination of nano/microcrystalline materials of different classes – from inorganic, to organic and biological compounds. The workshop included lectures and tutorials demonstrating the use of electron diffraction data for structure analysis.
Web address: https://acmm27.org/workshops/

- Workshop on 3D electron diffraction, Antwerp, Belgium, 30-31 May 2023

Number of Participants: 38

Level of involvement of SIG in the activity: organization, and lecturing by several SIG Members

ECA Individual Members registered with the SIG involved in the organizing committee: yes (Joke Hadermann, Tatiana Gorelik, Mauro Gemmi, Louisa Meshi, Tim Gruene)

ECA Individual Members registered with the SIG involved as lecturers: yes

SIG endorsed (SIG logo on the web page/leaflets): yes

Sponsored by ECA (Yes/ No)? no, not applied for

Short Description: Workshop on diverse aspects of 3D ED / MicroED, including method development and applications of the technique to various crystallographic problems. The aim of the workshop is to take a snapshot of the current state of the method, its achievements and problems. Although the workshop was not organized in the classical teaching format, it attracted scientists from complimentary fields willing to learn about the method and join the fast growing community.

Web address: https://ecaelectronsig.wordpress.com/schools/past/antwerp-2023/

- AIC school on Electron Crystallography, Pisa, Italy, 3rd - 6th July 2023

Number of Participants: 50 students participated

Level of involvement of SIG in the activity: several SIG4 members among the organizers and the teachers (Mauro Gemmi, Tatiana Gorelik, Enrico Mugnaioli, Tim Gruene, Petr Brazda, Gerhard Hofer)

ECA Individual Members registered with the SIG involved in the organizing committee: yes

ECA Individual Members registered with the SIG involved as lecturers: yes

SIG endorsed (SIG logo on the web page/leaflets): no logo, SIG4 was explicitly advertised at the closing ceremony

Sponsored by ECA (Yes/ No)? no

Short Description: It is the annual school organized by the Italian Crystallography Association (AIC) that this year was dedicated to electron diffraction. It was held in Pisa University and was divided in theoretical and practical sessions on 3D ED on inorganic, organic, macromolecular and 2D crystals. Other subject covered were texture and phase analysis by electron diffraction.

Web address: https://school2023.cristallografia.org/

- IUCr School on Electron Crystallography, Melbourne, Australia, 19-21 August 2023

Number of Participants: 40 students

Level of involvement of SIG in the activity: several SIG4 members among the organizers and the teachers (Hongyi Xu, Mauro Gemmi, Tatiana Gorelik, Ute Kolb, Lukas Palatinus, Louisa Meshi, Gerhard Hofer)

ECA Individual Members registered with the SIG involved in the organizing committee: yes

ECA Individual Members registered with the SIG involved as lecturers: yes

SIG endorsed (SIG logo on the web page/leaflets): no

Sponsored by ECA (Yes/ No)? no

Short Description: the school was organized as a satellite event to the 26th International Union of Crystallography Congress in Melbourne (22-29 August 2023). The main aim of the school was to educate postgraduate students and early career researchers about the latest progress in electron crystallography. The school covered two broad topics: 4D-scanning transmission electron microscopy and micro-electron diffraction, including convergent beam electron diffraction (CBED), quantitative CBED and scanning electron nanodiffraction (SEND), 4D scanning transmission electron microscopy (4D-STEM) and 3D electron diffraction (3D-ED) / micro electron diffraction (micro-ED).

Web address: https://sites.google.com/monash.edu/ecs2023/home

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- List of plenary / invited / teaching lectures of individual SIG members.

Plenary lecture: "*New possibilities in in situ and ex situ crystal structure determination based upon 3D ED*", ECSSC 2023: 18th European Conference on Solid State Chemistry, 9-12/07/2023, Czechia, **Joke Hadermann**

Invited lecture: "*In situ 3DED in gas and liquid environments for following structural evolutions during reactions*", 20th International Microscopy Congress, Korea, 9/9-15/9/2023, **Joke Hadermann**

Invited lecture: "*New possibilities in structure determination based upon 3D electron diffraction*", XXXIX Reunion Bienal de Quimica, Spain, 25-29/6/2023, **Joke Hadermann**

Invited teaching lecture: "*Teaching the basics of crystallography on a time budget*", 26th Congress and General Assembly of the IUCr, Australia, 22/8-29/8/2023, **Joke Hadermann**

Invited lecture: "*Electrons meet X-rays: Electron diffraction at the Centre for Chemical Structure Analysis*", Rigaku European Users' Meeting, Frankfurt/Main, 11th October 2022, **Tim Gruene**

Invited lecture: " *Single crystal diffraction with powders: the power of e-diffraction*", Excelsus 10 Years Celebration, PSI Villigen, 21st October 2022, **Tim Gruene**

Teaching lecture: "*Kinematical structural refinement with 3D ED data with SHELXL*", Electron Crystallography School, Pisa, 4th July 2023, **Tim Gruene**

Teaching lecture: "*Sample preparation and data collection for electron crystallography*", INSTRUCT-ERIC course, Oulu, 1st June 2023, **Tim Gruene**

Teaching lecture: "*Electron crystallography of 2D materials*", IFW winter school, 1-3 February, 2023, **Tatiana Gorelik**

Teaching lectures: "*Structure analysis of organic compounds*" and "*Disorder quantification and 2 crystals*", Electron Crystallography School, Pisa, 3-6 July 2023, **Tatiana Gorelik**

Teaching lecture: "*Crystallographic structure analysis with X-rays and electrons – common concepts, major differences*", Summer School VINCI, University of Silesia in Katowice, **Tatiana Gorelik**

Teaching lectures: "*3D ED data reduction and analysis*", "*Dynamical refinement*", "*Challenging problems and 3D ED data*", Electron Crystallography School, Pisa, 3-6 July 2023, **Petr Brazda**

Plenary lecture: "*Electron diffraction: a new tool for chemical analysis*", Annual Meeting 2023 of the Danish Chemical Society 17/08/2023, Copenhagen (Denmark), **Arianna Lanza**

Invited lecture: "Low-energy electron holography and coherent diffraction imaging" at "Mass spectrometry, electron microscopy, scanning probe microscopy" Conference Oxford, UK, 14/08/2022, **Tatiana Latychevskaia**

Invited lecture: "*Potentials of individual atoms by convergent beam electron diffraction (CBED)*" at "6th International Workshop on Models and Data for Plasma-Material Interaction in Fusion Devices (MoD-PMI 2023), 29/05/2023, Aachen, Germany, **Tatiana Latychevskaia**

Invited lecture: "*Crystal structure Determination of Small Molecules by 3D ED/MicroED*" The 73rd American Crystallographic Association Annual Meeting, Baltimore, USA, July 2023, **Hongyi Xu**

Invited lecture: "*MicroED - A Useful Tool for the Pharmaceutical Industry*" cryo-EM inauguration symposium at Sanofi, Paris, France, June 2023. **Hongyi Xu**

Invited lecture: "*Crystal Structure Determination by 3D ED/MicroED - from Materials to Protein*" ESTEEM3 European workshop on Advanced electron microscopy of ICT and quantum device material structures, Gothenburg, Sweden, May 2023. **Hongyi Xu**

Invited lecture: "*Structure characterization of small organic molecules*", ELDICO Scientific talk series, Online, Mar 2023. **Hongyi Xu**

Invited lecture: "*Crystal Structure Determination by 3D ED/MicroED - from Materials to Protein*" at the University of Queensland, Feb 2023, University of Sydney, July 2023, Australian National University, July 2023. **Hongyi Xu**

Invited lecture: "*Crystal Structure Determination by 3D ED/MicroED - from Materials to Protein*" at the 27th Australian Conference on Microscopy and Microanalysis, Australia, Jan 2023. **Hongyi Xu**

Invited lecture: "*Structure Determination of Macromolecules by MicroED*" at CCP4 Study Weekend, UK, Jan 2023. **Hongyi Xu**

Invited lecture: "*Microcrystal Electron Diffraction (MicroED) in MX*" Integrative structure biology, Helmholtz-Zentrum Berlin, Germany, Oct 2022. **Hongyi Xu**

Invited lecture: "*Computing optimal transport plans for molecular point cloud data: OT applications for drug resistance studies*", 2023 Joint Mathematics Meetings in Boston, MA in the AMS sponsored session on Current Progress in Computational Biomedicine, **Miranda Lynch**

Invited lecture: "*Seeing is believing: Visualizing submicron crystals as a first step towards direct protein sample preparation for microED experiments*", 2023 ACA meeting in Baltimore, MD, in the MicroED of Proteins session, **Miranda Lynch**

ELDICO Scientific talk series, "*Benefits of low dose electron diffraction*", **Stéphanie Kodjikian**, 27/10/2022 Online

Teaching lecture: "*Introduction to the determination of crystallographic structures by 3D electron diffraction*", Circle of JEOL microscopists, 26 sept 2023, **Stéphanie Kodjikian and Christophe Lepoittevin**

Tutorial: "*3D Electron diffraction, structure solution*", Circle of JEOL microscopists, 27 sept 2023, **Christophe Lepoittevin and Stéphanie Kodjikian**

Teaching lecture: "*Methods for phasing electron diffraction data*", IUCr2023 Electron Crystallography School, Aug. 18-21, Monash University, **Xiaodong Zou**

Invited lecture: "*Metal-organic frameworks - Fundamental science enabling transformative materials Nobel symposium in Chemistry (NS 193)*", Sept. 19-23, Karlskoga, Sweden, **Xiaodong Zou**

Invited lecture: "*Probing defects and disorders in nanoporous materials by electron crystallography*", IUCr2023, Aug 20-28, Melbourne, **Xiaodong Zou**

Invited lecture: "*Expanding the Horizons of Porous Materials Design and Applications"*, GRC Nanoporous Materials and Their Applications, August 6-11, 2023, Andover, NH, USA, High-throughput Electron Diffraction Advances the Development of Nanoporous Materials, **Xiaodong Zou**

Teaching lecture: "*Advances in electron crystallography techniques and their applications for structure determination and phase analysis",* The 14th K.H. Kuo Summer School on Electron Microscopy and Crystallography, July 9-13, 2023, Shenyang, China, **Xiaodong Zou**

Teaching lecture: "*Applications of advanced electron diffraction in crystallography - from structure determination of unknown crystals to high-throughput polycrystalline phase analysis",* The 14th K.H. Kuo Summer School on Electron Microscopy and Crystallography, July 9-13, 2023, Shenyang, China, **Xiaodong Zou**

Invited lecture: "*Emerging electron diffraction techniques in crystallography – from ab initio structure determination to high-throughput phase analysis",* Distinguished iNANO lecture, May 26, Aarhus University, Denmark, **Xiaodong Zou**

Invited lecture: "*3D Electron Crystallography: Past, Present, and Future",* Eleventh Sweden Japan Academic Seminar (11th SJAN), March 14, Stockholm, **Xiaodong Zou**

Plenary lecture: "*New electron crystallographic techniques for structural elucidation of porous materials",* 34th German Zeolite Conference, Feb. 21 – 23, Vienna, **Xiaodong Zou**

Invited lecture: *Automated and high-throughput electron diffraction techniques for the development of novel nanoporous materials.* 14th International Workshop on Advanced Materials, Feb 18-21, RAK, UAE, **Xiaodong Zou**

Invited lecture: *MicroED for structural biology - what can we learn from structural analysis of small molecules?,* Advances and Challenges in cryoEM Summit, Jan. 17-20, UCLA, Los Angels, USA, **Xiaodong Zou**

Invited lecture: "*Discovery of New Nanoporous Materials Advanced by Electron Crystallography",* 26th Solvay Conference on Chemistry - Chemistry Challenges, Nov. 16-19, Brussels, Belgium, **Xiaodong Zou**

Invited lecture: "*The Breakthrough of Emerging Electron Diffraction Techniques in Crystallography",* 2nd Princeton-Nature Conference: Frontiers in Electron Microscopy for the Physical and Life Sciences, September 28-30, 2022, Princeton, **Xiaodong Zou**

Plenary lecture: *"The Impacts of Advanced Electron Diffraction Techniques for Structural Elucidation of Metal-Organic Frameworks and Covalent Organic Frameworks"*, The 8th International Conference on Metal-Organic Frameworks and Open Framework Compounds (MOF2022), September 3-7, 2022, Dresden, **Xiaodong Zou**

Keynote lecture: "*My journey to become a scientist for the development of electron crystallography",* Young Investigator Symposium MOF2022, September 3, 2022, Dresden, **Xiaodong Zou.**

- Resources

PDFs and tutori'al data of several lectures are available online:
https://homepage.univie.ac.at/tim.gruene/research/seminars

- List SIG officers

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