

SIG4 activity report January 2021-August 2022

- **Editorial activity of SIG members**

In 2022 IUCrJ has launched a new section on Electron Crystallography. Xiaodong Zou has been appointed as Main Editor. Mauro Gemmi, Louisa Meshi, Peter Nellist, Jose Rodriguez and Junliang Sun are appointed as co-editors.

MDPI Special Issue in Symmetry: Electron Diffraction and Structural Imaging

Volume I:

https://www.mdpi.com/journal/symmetry/special_issues/Electron_Diffraction_Structural_Imaging

No of Accepted Publications: 9 (Issue Closed)

Volume II:

https://www.mdpi.com/journal/symmetry/special_issues/Electron_Diffraction_Structural_Imaging_I

No of Accepted Publications: As of now 2, (Deadline 31st Dec, 2022)

Guest Editors: Partha Pratim Das, Arturo Ponce-Pedraza, Enrico Mugnaioli, Stavros Nicolopoulos

- **Organization of ECM33**

SIG4 representative – Andy Stewart

- **SIG4 mail list**

26 posts on events related to electron crystallography within the last year, 56 members on the list.

Responsible - Jérôme Pacaud jerome.pacaud@univ-poitiers.fr

Organization of dedicated schools / workshops

- **The 41st Ad Hoc Workshop on Jana: Electron diffraction, 24-25 March 2021, Broadcasted from Prague, Czech Republic**

Number of Participants: 80

Level of involvement of SIG in the activity: organization, lecturing (Lukáš Palatinus, Mariana Klementová, Petr Brázda)

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: 2-day online workshop combining lectures and practical sessions. Topics covered: theoretical introduction to electron crystallography, experimental details and data collection, data processing methods for electron crystallography, preparation of input for Jana2020, kinematical structure refinement from electron diffraction data, structure refinement using dynamical diffraction theory.

<http://jana.fzu.cz/w041.html>

- **An Introductory Course to Three-Dimensional Electron Diffraction, 12 - 15 April 2021, online.**

Number of participants: >400 registered participants

Level of involvement of SIG in the activity: organization, lecturing (Zhehao Huang, Hongyi Xu, Tom Willhammar, Xiaodong Zou)

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

The course was dealing with 3D ED data collection, processing and use for structure elucidation with an emphasis on the theory of electron diffraction and the use of computer programs for processing 3DED data and determining crystal structures. The course included live demonstration 3DED data collection on TEM and practical sessions on data analysis and processing software, including REDp, XDS and SHELX.

<https://www.mmk.su.se/3ded-course/welcome>

- **Electron Crystallography School: 3D Electron Diffraction/MicroED - Uniting Small Molecule and Macromolecular Crystallography, 11 – 13 August 2021, satellite of the 25th IUCr congress, online /hybrid**

Number of Participants: 202

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): no

Sponsored by ECA (Yes/ No)? no

Short Description: School on 3D electron diffraction/MicroED techniques and how to apply them for structure determination of nano/microcrystals too small for X-ray diffraction. The topics covered inorganic compounds, pharmaceuticals and proteins. The school included both lectures and practical sessions.

<http://www.xray.cz/iucr/workshops/tabor/default.htm>

- **Workshop on ePDF, 1-2 September 2021, satellite of the 25th IUCr congress, online**

Number of Participants: 55

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): no

Sponsored by ECA (Yes/ No)? no

Short Description: The workshop comprised two and a half days of lectures by renown international researchers complemented by ample opportunities for discussions. The topical focus is devoted to electron scattering phenomena beyond Bragg diffraction, calculation of pair distribution function from electron diffraction data (ePDF), interpretation of the data and the strength and limitation of the method.

<https://www.uni-ulm.de/einrichtungen/hrem/epdf/epdf/>

The third edition of the CrystElec school, 11-15 October 2021, Grenoble France

Number of Participants: 15

Level of involvement of SIG in the activity: organization, lecturing (Damien Jacob, Edgar Rauch, Muriel Veron, Philippe Boulay, Pascal Roussel, Lukas Palatinus)

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: Bringing together fifteen participants and eight lecturers, the training focused on the determination of structures and microstructures at the nanometric scale by electron diffraction in a transmission electron microscope (TEM). After a basic review of geometrical optics and crystallography, the recent developments associated with the use of new data acquisition and

analysis techniques such as electron precession, electron tomography and phase and orientation mapping were presented.

- **6th ECA Lunch webinar 9th of December 2021, online**

Hosea Nelson: "Applications of electron diffraction in organic chemistry"

Abstract: In this talk I will discuss our groups efforts to use electron diffraction to solve problems in organic chemistry. We will specifically discuss applications in natural products science, including the structural re-assignment of well-known natural products and the discovery of new natural products. We will also discuss applications in the structural determination of organometallic complexes, reactive intermediates, and functional materials. A brief survey of opportunities for future discoveries and advances will also be discussed.

- **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.

<https://ecs2022.sciencesconf.org/>

CrysAC Micro- and nano-diffraction for cultural heritage, 23rd August, 2022, Satellite to ECM33, Louvre, France

Number of Participants: 40

Level of involvement of SIG in the activity: No

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 present workshop covers lectures by the scientists from research institutions, museums, and conservation bodies, in order to illustrate state-of-the-art applications of diffraction techniques in the sub-micron spatial resolution. Recent instrumental and methodological advances, mainly based on electron diffraction and synchrotron radiation, are opening novel fields of research on cultural heritage materials, to understand chemico-physical processes and structural transformations with unprecedented spatial resolutions.

Individual lectures of SIG members (plenary, invited, teaching)

ELDICO webinar series, online

Lecture: "Demanding crystallographic problems of inorganics solved by 3D-ED – Benefits of STEM-ADT", Ute Kolb, January 2021

Lecture: "Absolute structure determination from 3D electron diffraction", Lukas Palatinus & Paul Klar, April 2021

Lecture "Revealing Invisibles: The Power of 3D-ED for Studying MOF Nanocrystals", Zhehao Huang, June 2021

Lecture: "Characterization of nano-sized intermetallics in Al-alloys and in high entropy alloys", Louisa Meshi, February 2022

Lecture: "When is a particle a crystal - electron diffraction will tell", Andy Stewart, July 2022.

Sustainable Chemistry Lecture webinar series

Lecture: Advanced transmission electron microscopy techniques for developing novel materials for sustainable chemistry", Xiaodong Zou, 20 May, 2021.

8th Conference of the Federation of European Zeolite Associations (FEZA2021 virtual) 5-9 July, 2021, online

Plenary lecture: "The impacts of electron crystallographic methods for structural studies of porous materials", Xiaodong Zou

28th Congress of the Brazilian Society of Microscopy and Microanalysis, 12 to 15 July 2021, online

Invited lecture: "3D Electron Diffraction - a universal tool for structure characterization of nanocrystals", Tatiana Gorelik

ACA 2021 annual meeting, July 31-August 5, online

Invited lecture: "Structural analysis of polymorphs of small organic molecules by 3D ED/MicroED" Hongyi Xu

Invited lecture: "Dynamical refinement: The way to improved fit, accurate structure models and absolute structure from 3D ED data", Lukas Palatinus

Invited lecture: "A simple pressure-assisted method for MicroED specimen preparation", Jingjing Zhao

Invited lecture: "DIALS data processing for MicroED" David Waterman

M&M 2021, 2-5 August 2021, online

Invited lecture: "Unifying 3D electron diffraction and serial electron diffraction into a high-resolution, high-accuracy and high-throughput structural analysis technique", Xiaodong Zou

25th IUCr Congress, 14-22 August 2021, Prague, Czech Republic, hybrid

Invited lecture: "3D electron diffraction on nanoparticles with a complex structure", Mauro Gemmi

Invited lecture: "Reliable structure determination of K-intercalated RuCl₃ nanoflakes by 3D electron crystallography and multivariate analysis of fused EELS and EDX data", Maria Roslova

Key note lecture: "Electron Crystallography of Molecular Crystals", Lukas Palatinus

Keynote lecture: "Electron Crystallography – from slow 2D of simple structures to rapid crystal structure determinations in 3D of very complex structures", Sven Hovmöller

Keynote lecture: "The development of automated diffraction tomography", Ute Kolb

Invited lecture: "Strategies for structure solution of small-molecule organics by 3D ED using a small beam", Enrico Mugnaioli

Invited lecture: "Structure Determination of Biomolecules by 3D Electron Diffraction", Hongyi Xu

Invited lecture: "X-Ray Powder Diffraction and Electron Single Crystal Diffraction – two techniques for structure analysis of nanocrystals", Tatiana Gorelik

Invited lecture: "In the Age of Electrons, Do We Still Need Powder Diffraction?", Stef Smeets

Invited lecture: "Local Structure Analysis by Pair Distribution Function Obtained from a TEM", Cheuk-Wai Tai

Invited lecture: "Following structure evolution of SrFeOx in redox reactions using in situ 3D electron diffraction", Maria Batuk.

Q-SORT International Conference on Quantum Imaging and Electron Beam Shaping, 1-3 September 2021, online.

Invited lecture: "Recent results in 3D wavefront modulation and quantum mechanical detection", Tatiana Latychevskaia

SSRL Users' Meeting 2021, 21 September 2021, online

Invited lecture: "Electron crystallography for X-ray crystallographers", Tim Gruene

International Workshop on Total Scattering for Nanotechnology ToScal'And, 20 – 24 September, 2021, Granada, Spain

Lecture: "Introduction to Electron Diffraction and e-PDF methods", Tatiana Gorelik

RIGAKU: Electron Diffraction (MicroED/3D ED) Workshop, 27-28 October 2021, online

Lecture: "Concept, implementations and potentials of 3DED", Enrico Mugnaioli

Lecture: "3D ED/MicroED for structure determination of porous materials and pharmaceutical compounds", Hongyi Xu

Lecture: "Specifics of structure analysis from 3DED data", Lukas Palatinus

American Institute of Chemical Engineers Annual Meeting, 15-19 November, 2021, Boston, USA.

Invited lecture: "Insights into Structural Details of Zeolites via Three-Dimensional Electron Diffraction", Zhehao Huang

25th NECZA (Northeast Corridor Zeolite Association) annual meeting, 3 December, 2021, online

Invited lecture: "Advanced electron crystallographic techniques for structure elucidation and discovery of novel zeolites", Xiaodong Zou

34. Irsee Naturstofftage 2022, 18th February, 2021, online

Invited lecture: "Structure Determination of Natural Products with Electron Crystallography", Tim Gruene

Seminar series of the Physikalische Gesellschaft Zürich, 10 March, 2022, Switzerland

Invited lecture: "Ptychography - scanning coherent diffraction imaging technique, principles and applications", Tatiana Latychevskaia

Webinar series at the IIT Dehli student chapter of OPTICA (formerly OSA) / SPIE, February 2022, online

Invited lecture: "Phase retrieval for coherent imaging", Tatiana Latychevskaia

Diamond Diffraction Meeting, 23rd March 2022

Invited lecture: "Not only X-rays: the level of detail extracted by the JUNGFRU detector with electron diffraction", Tim Gruene

SALVE 2D22 Symposium, 4-7 April, 2022, Ulm

Invited lecture: "Convergent beam electron diffraction of two-dimensional materials", Tatiana Latychevskaia

BCA Spring Meeting, 11-14th April 2022

Plenary lecture: "3D electron crystallography: past, present and future", Xiaodong Zou

Invited lecture: "Instrumental requirements for electron crystallography are less demanding than you might think", Tim Gruene

NanED Workshop I - Data processing and structure refinement, 25 - 27 May, 2022, Prague

Lecture: "Structure solution and refinement – theoretical aspects" Tim Gruene

Lecture: "Structure refinement from 3D ED data with SHELX" Tim Gruene

Lecture: "Structure refinement from 3D ED data with Jana2020", Lukas Palatinus

Lecture: "Experimental data collection strategies", Mauro Gemmi, Philippe Boullay

Lecture: "Data processing – theoretical aspects", Lukas Palatinus

Lecture: "Data processing with XDS", Hongyi Xu

Lecture: "Data processing with PETS2", Petr Brázda

Lecture: "Specimen preparation of macromolecular crystals", Gerhard Hofer, Hongyi Xu

Lecture: "TEM hardware, data collection and data pre-processing", Eric van Genderen

Lecture: "Data processing and structure determination for macromolecules", Gerhard Hofer

Webinar of the French Chemical Society, division of Solid State Chemistry, 9th June 2022, online

Lecture: "3D ED: a powerful structural characterization tool for solid state chemistry", Philippe Boullay

The 9th International Charge Density Meeting – ICDM9, 12-16 June, 2022, Aarhus, Denmark

Lecture: "Subatomic Features of the Electrostatic Potential in 3D Electron Diffraction Data", Petr Brazda

Biennial of the Spanish Chemistry Society, 29th June 2022

Invited lecture: "Progress of coking in zeolite ZSM5 studied with electron diffraction", Tim Gruene

IZC (International Zeolite Conference) school, 1-2 July 2022, Valencia, Spain

Lecture : "Structure determination of microporous materials at the atomic scale using electron microscopy", Tom Willhammar

20th International Zeolite Conference, 3-8 July, 2022, Valencia, Spain

Plenary lecture : "The impacts of New Electron Crystallographic Techniques on Developing Nanoporous Materials", Xiaodong Zou

Summer Course on Neutrons, Electrons and X-Ray techniques. Satellite event of SETN 2022, 21st-22nd July 2022, Almeria Spain

Lecture: "3D Electron diffraction", Mauro Gemmi.

VINCI – Interdisciplinary International Silesian Summer School, 4-22 July 2022, University of Silesia in Katowice, Poland

Lecture: "Crystallographic structure analysis with X-rays and electrons – common concepts, major differences", Tatiana Gorelik

Lecture: "Obtaining information from electron diffraction patterns", János Lábár

Lecture: "Analysis of the disordered structure of materials on the basis on the X-ray electron diffraction", Maciej Zubko

The 6th Stanisław Gorczyca European School on Electron Microscopy and Tomography, 12-15 July, 2022, Krakow, Poland

Lecture: "Conventional electron diffraction and 3DED", Joke Hadermann

To be sent to Jan Dohnalek by the end of July 2022