

Monday, August 25

17:00 Opening ceremony

Ambassador of Ukraine to Poland – Vasyl Bodnar

Mayor of the City of Poznań - Jacek Jaśkowiak

President of the European Crystallographic Association – Arie van der Lee

Chair of the ECM35 Program Committee – Roman Gladyshevskii

Chair of the ECM35 Organising Committee – Maciej Kubicki

17:30 Plenary lecture 1

Chair: Roman Gladyshevskii (Ivan Franko National Univ. Lviv, Ukraine)

Crystallography – a subject that constantly reinvents itself

Sven Lidin (Lund Univ., Sweden)

18:30 Perutz Prize

Chair: Jan Dohnálek (ECA Vice-President)

My life as a curious crystallographer

Gilberto Artioli (Univ. Padova, Italy)

19:30 Welcome to Ukraine

20:00-22:00 Welcome reception

Tuesday, August 26

8:30 - 9:15 Keynote lectures:

8:30 – 9:15 KEYNOTE 1 (1.E)

Modulation and modularity in natural and synthetic sulfosalts

Berthold Stöger (TU Vienna, Austria)

Chair: Anna Makal (Univ. of Warsaw, Poland)

8:30 – 9:15 KEYNOTE 2 (1.G)

Crystallochemistry underneath function: in situ power diffraction at work

Simona Galli (Univ. Insubria, Como, Italy)

Chair: Chiara Massera (Univ. of Parma, Italy)

8:30 – 9:15 KEYNOTE 3 (1.B)

George Sheldrick's SHELX: success for all

Isabel Uson (IMB Barcelona, Spain)

Chair: Michal Chodkiewicz (Univ. of Warsaw)

9:45 MS5 – Structural studies in enzymology (1.E)

Chairs: Isabel Bento (MAX IV, Lund, Sweden), Matthias Bochtler (IIMCB, Warsaw, Poland)

9:45 MS5_01 / invited speaker

High-precision, high-accuracy macromolecular crystallography

Ashwin Chari (MPI Multidisciplinary Sciences, Göttingen, Germany)

10:15 MS5_02 / invited speaker

Time-resolved X-ray diffraction studies of enzymatic reactions

Richard Neutze (Univ. Gothenburg, Sweden)

10:45 MS5_03

Structure correlation analysis of the nucleophilic attack in the three classes of L-asparaginases

Mariusz Jaskolski (Adam Mickiewicz Univ., Poznan, Poland)

11:05 MS5_04

Awakening Striga: cooperative strigolactone perception by the E3 ubiquitin ligase–receptor–substrate complex

Stefan Arold (KAUST, Thuwal, Saudi Arabia)

11:25 MS5_05

Advanced cryo-trapping time-resolved crystallography: SPITROBOT-2 enables investigation of protein dynamics with millisecond time resolution

Maria Spiliopoulou (UKE, Hamburg, Germany)

9:45 MS9 – The new role of experiments in the age of protein fold prediction (1.G)

*Chairs: Charles Ballard (STFC Rutherford Appleton Lab., United Kingdom),
Nicholas Pearce (Linköping Univ., Sweden)*

9:45 MS9_01 / invited speaker

Validating protein structures in the AlphaFold 3 Era: A contact map-based approach with konkit-validate

Adam Simpkin (Univ. Liverpool, United Kingdom)

10:15 MS9_02 / invited speaker

Validation of symmetric protein assemblies predicted by SymProFold

Christoph Grninger (Univ. Graz, Austria)

10:45 MS9_03

Addressing quality gaps and enabling data interoperability of nucleic acid structures

Bohdan Schneider (IBT-CAS, Vestec, Czech Republic)

11:05 MS9_04

Racemic crystal structure of a synthetic DNA hairpin with diquinoline linker

Pradeep Mandal (ISTA, Klosterneuburg, Austria)

11:25 MS9_05

Bacterial toxin interaction with human glycolipid: Structure of *Pseudomonas aeruginosa* lectin LecA/galactose complex using neutron macromolecular crystallography

Théodore Arnaud (ILL, Grenoble, France)

9:45 MS22 – Short-range order as seen by different techniques (1.B)

Chairs: Giovanni Orazio Lepore (Univ. Florence, Italy), Wojciech Sławiński (Univ. Warsaw, Poland)

9.45 MS22_01 / invited speaker

Coupling X-ray diffuse scattering and spectroscopy to explore the local structure of hollandites

Marta Morana (Univ. Florence, Italy)

10.15 MS22_02 / invited speaker

Determining short – and long-range aluminium ordering in zeolite structures

Przemysław Rzepka (CAS, Prague, Czech Republic)

10.45 MS22_03

Lack of long-range order in ‘relaxor’ ferroelectric $\text{NH}_4\text{Zn}(\text{HCOO})_3$: diffuse and inelastic scattering study

Johnathan Bulled (ESRF, Grenoble, France)

11.05 MS22_04

Investigating trimeron dynamics and lattice instabilities in Magnetite

Benjamin Fahl (ETH Zurich, Switzerland)

11.25 MS22_05

Local distortions and orbital disorder in $\text{Ce}_{0.5}\text{Ba}_{0.5}\text{MnO}_3$ as seen by neutron PDF

Elizabeth Arnold (Univ. Warwick, Coventry, United Kingdom)

9:45 MS25 – Supramolecular interactions behind crystal engineering (1.C)

Chairs: Leonard Barbour (Univ. Lincoln, United Kingdom), Kreso Bucar (Univ. College London, United Kingdom), Agnieszka Janiak (Adam Mickiewicz Univ., Poznan, Poland)

9:45 MS25_01 / invited speaker

Non-covalent interactions in silver(I) mixed-ligand complexes

Susan Bourne (Univ. Cape Town, South Africa)

10:15 MS25_02 / invited speaker

A journey into the complex world of fampridine salts

Riccardo Montis (Univ. Urbino Carlo Bo, Italy)

10:45 MS25_03

Structure and coordination chemistry of some aminopyrazoles, 1,3-diazocanes, and fused dipyrazoloheterocycles

Louise Dawe (Wilfrid Laurier Univ., Waterloo, Canada)

11:05 MS25_04

Supramolecular Approaches to Functional Cocrystal Design

Ranjit Thakuria (Gauhati Univ., India)

11:25 MS25_05

Desmotropy, polymorphism, and packing relationships of 5-monosubstituted derivatives of barbituric acid

Thomas Gelbrich (Univ. Innsbruck, Austria)

9:45 MS33 – Nucleation and crystal growth (1.D)

Chairs: Filipa Castro (Univ. Minho, Braga, Portugal), José Gavira (IACT-CSIC, Granada, Spain)

9:45 MS33_01 / invited speaker

**Exploring nucleation pathways across diverse physicochemical environments:
Unveiling new strategies to modulate and optimize biomolecular crystallization**
Christian Betzel (Univ. Hamburg, Germany)

10:15 MS33_02 / invited speaker

**Microfluidics and photonics for the study of crystalline nucleation: probing
beyond conventional spatiotemporal barriers**
Isaac Rodríguez-Ruiz (LGC-CNRS, Toulouse, France)

10:45 MS33_03

**Beauty and complexity of calcium carbonate precipitation: optical microscopy
and in situ Raman microspectroscopy characterization**
Natercia Barbosa (Univ. Geneva, Switzerland)

11:05 MS33_04

**Using phase diagrams with microseeding to prepare crystal samples for
advanced data collection techniques**
P. D. Shaw Stewart (Douglas Instruments Ltd., Hungerford, United Kingdom)

11:25 MS33_05

**Diffusion-controlled crystallization inspired by biomineralization, and its
bioapplications**
Sung Ho Yang (KNUE, Cheongju, Korea)

9:45 MS41 – Total scattering and Pair Distribution Function analysis (1.F)

Chairs: Nicola Dengo (Univ. Insubria, Varese, Italy), Adam Sapnik (Univ. Copenhagen, Denmark)

9:45 MS41_01 / invited speaker

Electron Pair Distribution Function analysis in the scanning TEM for probing nanoscale heterogeneity in amorphous and crystalline polymers and metal-organic frameworks

Sean Collins (Univ. Leeds, United Kingdom)

10:15 MS41_02 / invited speaker

Ultrafast Pair Distribution Function as a probe of hidden states in quantum materials

Emil Bozin (Inst. Physics Belgrade, Serbia)

10:45 MS41_03

Benchmarking the 3D- Δ PDF using in-house X-ray sources

Karl Juul (Aarhus Univ., Denmark)

11:05 MS41_04

Local structure of Ammonia Borane described using PDF method

Anna Piekara (Univ. Warsaw, Poland)

11:25 MS41_05

ePDF mapping: a new tool for nanometer scale analysis of amorphous materials

Partha Pratim Das (NanoMEGAS SRL, Brussels, Belgium)

14:00 MS2 – Room temperature and serial crystallography and dynamics (1.E)

Chairs: Sebastian Günther (DESY, Hamburg, Germany), Dean Lang (MAX IV, Lund, Sweden)

14:00 MS2_01 / invited speaker

Tracking the structural dynamics of cytochrome c oxidase

Gisela Brändén (Univ. Gothenburg, Sweden)

14:30 MS2_02 / invited speaker

Photoenzyme dynamics studied using serial femtosecond crystallography

Thomas Barends (MPI Medical Research, Heidelberg, Germany)

15:00 MS2_03

Mechanistic insights into heme iron photoreduction: influence of temperature on redox and structural states

Vera Pfanzagl (BOKU Univ., Vienna, Austria)

15:20 MS2_04

Probing the modulation of enzyme kinetics by multi-temperature, time-resolved serial crystallography

Eike Schulz (UKE, Hamburg, Germany)

15:40 MS2_05

MicroMAX – Advanced Beamline for Serial Crystallography and Time-Resolved Studies

Monika Bjelcic (MAX IV, Lund, Sweden)

14:00 MS10 – Structure-property relationships in materials (1.G)

Chairs: Volodymyr Pavlyuk (Ivan Franko National Univ., Lviv, Ukraine), Pavlo Solokha (Univ. Genova, Italy)

14:00 MS10_01 / invited speaker

Relating structure and spin crossover properties in Hofmann complexes

Hanna Boström (Stockholm Univ., Sweden)

14:30 MS10_02 / invited speaker

Amorphous GeTe: Structure vs phase change memory properties

Maksym Yarema (ETH Zurich, Switzerland)

15:00 MS10_03

Engineering thermochromism in low-dimensional perovskites through halogen bonding

Gabriella Cavallo (Polytechnic Univ. Milan, Italy)

15:20 MS10_04

Lively crystals – on the mechanism of thermally induced structural adjustments in elastically adaptable coordination polymers

Mateja Pisacic (Univ. Zagreb, Croatia)

15:40 MS10_05

Structure-property interplay in $\text{Cu}_6\text{Te}_{3-x}\text{S}_{1+x}$: An analytical approach to thermoelectric optimization

Krzysztof Wojciechowski (AGH Univ. Kraków, Poland)

14:00 MS18 – Novel advances in quantum crystallography (1.B)

Chairs: Florian Kleemiss (RWTH-Aachen, Germany), Anna Krawczuk (Univ. Göttingen, Germany)

14:00 MS18_01 / invited speaker

Some of the recent history of quantum crystallography

Simon Grabowsky (Univ. Bern, Switzerland)

14:30 MS18_02 / invited speaker

Dynamic quantum crystallography: Principles, latest developments, and applications

Anna Hoser (Univ. Warsaw, Poland)

15:00 MS18_03

Investigation of the anharmonic atomic motion in molecular crystals using the GFN2-XTB molecular dynamics approach

Michael Patzer (MPI-Mülheim, Germany)

15:20 MS18_04

Reconstruction of polarization and correlation effect in molecular crystals through the lens of one-electron reduced density matrix

Sizhuo Yu (Paris-Saclay Univ., France)

15:40 MS18_05

Insights into atomic bonding from dynamical multipole refinement of three-dimensional electron diffraction data

Ashwin Suresh (FZU-CAS, Prague, Czech Republic)

14:00 MS32 – Designing the void: structural mastery in advanced porous materials (1.C)

Chairs: Volodymyr Bon (TU Dresden, Germany), Felipe Gandara (ICMM-CSIC, Madrid, Spain)

14:00 MS32_01 / invited speaker

Metal-Organic Frameworks: crystallographic explorations of porosity and functionality

Valentina Colombo (Univ. Milan, Italy)

14:30 MS32_02 / invited speaker

Azolate coordination networks for adsorptive purification of light hydrocarbons

Soumya Mukherjee (Univ. Limerick, Ireland)

15:00 MS32_03

Complementary tools for in situ analysis of porous materials – some perspectives

Len Barbour (Univ. Lincoln, United Kingdom)

15:20 MS32_04

Unique gas adsorption properties of the first Porous Ionic Packings (PIPs)

Yaroslav Filinchuk (Univ. Catholique Louvain, Belgium)

15:40 MS32_05

3-Dimensional electron diffraction and in-situ activation of metal organic frameworks

Calum Sangster (Univ. Edinburgh, United Kingdom)

14:00 MS34 – AI in crystallography (1.D)

Chairs: Arnt Kern (Bruker AXS, Karlsruhe, Germany), Rosanna Rizzi (IC-CNR, Bari, Italy)

14:00 MS34_01 / invited speaker

Artificial intelligence in crystallography: Navigating big data challenges

Detlef Hofmann (CRS4, Cagliari, Italy)

14:30 MS34_02 / invited speaker

PhAI: Neural network for structure determination

Anders Østergaard Madsen (Univ. Copenhagen, Denmark)

15:00 MS34_03

Detecting symmetry groups in crystallographic tilings

Bartosz Naskrecki (Adam Mickiewicz Univ., Poznań, Poland)

15:20 MS34_04

Deep Learning for smart sample alignment

Anna Lübben (Bruker AXS, Karlsruhe, Germany)

15:40 MS34_05

What I learned about structure from artificial intelligence

Simon Billinge (Columbia Univ., New York, USA)

14:00 MS48 – Potential of online courses in crystallography (1.F)

Chairs: Kamil Dziubek (Univ. Vienna, Austria), Gemma de la Flor Martin (KIT, Karlsruhe, Germany)

14:00 MS48_01 / invited speaker

Online learning with the Cambridge Structural Database (CSD)

Ilaria Gimondi (CCDC, Cambridge, United Kingdom)

14:30 MS48_02 / invited speaker

Fourier goggles: on! Rediscovering crystallography through the beauty of frequencies

Stefano Canossa (ETH Zurich, Switzerland)

15:00 MS48_03

Crystallography and crystallization MOOC: Empowering secondary schools teachers through online learning

Pilar Garcia-Orduña (Univ. Zaragoza, Spain)

15:20 MS48_04

Post-COVID extension of an online crystallography school

Mathias Meyer (Rigaku Polska, Wrocław, Poland)

15:40 MS48_05

Insights into the community-driven effort behind organizing accessible national crystallography courses by the Polish Young Crystallographers

Daniel Tchoń (FZU-CAS, Prague, Czech Republic)

16:30 – 17:15 Keynote lectures:

16:30 – 17:15 KEYNOTE 4 (1.E)

Structural insight into the complex regulation of the Calvin-Benson cycle

Simona Fermani (Univ. Bologna, Italy)

Chair: José Gavira (IACT-CSIC, Granada< Spain)

16:30 – 17:15 KEYNOTE 5 (1.G)

Electron density and chemical bonding in intermetallic compounds

Juri Grin (MPI Chemical Physics of Solids, Dresden, Germany)

Chair: Gabriella Cavallo (Polytechnic Univ. of Milan, Italy)

16:30 – 17:15 KEYNOTE 6 (1.B)

Application of crystal engineering tools for the design of multiphase formulations for food and pharmaceuticals

Elena Simone (Politecnico Torino, Italy)

Chair: Paulina Dominiak (Univ. of Warsaw, Poland)

17:15 Remembering George Sheldrick (1.E)

Chairs: Isabel Uson (IBMB-CSIC, Barcelona, Spain), Regine Herbst-Irmer (Univ. Göttingen, Germany)

18:00 Sheldrick Prize

Chair: Marijana Đaković (Univ. Zagreb, Croatia)

Dynamic X-ray diffraction for the design of functional photoswitches

Lauren E. Hatcher (Cardiff Univ., Great Britain)

Dr Lauren E Hatcher, Royal Society University Research Fellow (URF) at Cardiff University, is awarded the 2025 George Sheldrick Prize in recognition of her pioneering contributions to time-resolved crystallography and the structural study of photoactive materials. Dr Hatcher has developed and applied advanced crystallographic techniques to capture dynamic photoinduced processes in crystals, enabling 3D structural visualisations across timescales from minutes to picoseconds. Her work offers transformative insights into photoinduced ferroelectricity and holds significant promise for next-generation solar energy materials.

With a strong early-career publication record, Dr Hatcher has demonstrated exceptional scientific leadership. She has also made major contributions to crystallographic education and outreach, including teaching at European Crystallography Schools and serving in multiple leadership roles within the British Crystallographic Association. Her collaborative network spans UK and international institutions, and her research continues to advance the field of crystallography by introducing the dimension of time into her crystallographic studies.

Dr Hatcher's work exemplifies the spirit of innovation and excellence celebrated by the George Sheldrick Prize.

19:30 Concert at AMU Hall

AMU Hall (Aula UAM), Wieniawskiego 1, Poznań



Concert Programme

Masterpieces Known and Unknown

Fryderyk Chopin (1810–1849)

Polonaise in A-flat major, Op. 53

Waltz in C-sharp minor, Op. 64 No. 2

Franz Xaver Scharwenka (1850–1924)

Polish Dance

Juliusz Zarębski (1854–1885)

Piano Quintet in G minor, Op. 34

Performers

Marcin SUSZYCKI – violin

Ewa KOZIEŁ-SUSZYCKA – violin

Dominik DĘBSKI – viola

Józef CZARNECKI – cello

Michał FRANCUZ – piano

Hosting the concert

Karolina Kaźmierczak

21:00 Young Crystallographers mixer!



**The Programme Committee and the Organizing Committee
of the 35th European Crystallographic Meeting**

invite you to the
Young Crystallographers mixer!

Join us at the Blue Note Jazz Club

79 Kościuszki Street, Poznań

on Tuesday, 26 August.

The party kicks off at 9:00 pm.

Wednesday, August 27

8:30 - 9:15 Keynote lectures:

8:30 – 9:15 KEYNOTE 7 (1.E)

Weak, noisy and uninteresting

Nicholas Pearce (Linköping Univ., Sweden)

Chair: Ronan Keegan (STFC Rutherford Laboratory, Didcot, United Kingdom)

8:30 – 9:15 KEYNOTE 8 (1.G)

A Journey to the Nanoscale through Electron Diffraction

Sergi Plana Ruiz (Univ. Rovira i Virgili, Tarragona, Spain)

Chair: Anna Hoser (Univ. of Warsaw, Poland)

8:30 – 9:15 KEYNOTE 9 (1.B)

Towards an individualized path to self-learning in integrative structural biology

Marie-Hélène Le Du (CEA, Saclay, France)

Chair: Mateja PISAČIĆ (University of Zagreb, Croatia)

9:45 MS1 – Nucleic acids, proteins – structures, interactions (1.E)

Chair: Martin Hällberg (Karolinska Institutet, Stockholm, Sweden)

9:45 MS1_01 / invited speaker

New aspects of DNA recognition by plant WRKY transcription factors revealed by structural and functional study

Marta Grzechowiak (IBCH-PAN, Poznań, Poland)

10:15 MS1_02 / invited speaker

Unprecedented nuclease activity explained by structure – where one bond matters

Jan Dohnálek (IBT-CAS, Vestec, Czech Republic)

10:45 MS1_03

Crystal Structure of the TREX1–DNA Mimic Foldamer Complex: A Novel Inhibition Mechanism of the First Foldamer-Based Inhibitor Targeting the Cancer Immunotherapeutic Protein

Yu-Yuan Hsiao (NYCU, Hsinchu, Taiwan)

11:15 MS1_04

Naphthyridine carbamate dimer ligand induces formation of Z-RNA-like fold of disease-related RNA and serves as a molecular glue for crystal lattice formation

Martyna Mateja-Pluta (IBCH-PAN, Poznań, Poland)

9:45: MS11 – Molecular structures with material properties (1.G)

Chairs: Marlena Gryl (Jagiellonian Univ., Kraków, Poland), Rebecca Scatena (Diamond LS, Didcot, United Kingdom)

9:45 MS11_01 / invited speaker

Understanding and tuning the electronic structure of covalent organic frameworks

Michelle Ernst (Univ. Zurich, Switzerland)

10:15 MS11_02 / invited speaker

Crystal Engineering of bismuth iodide derivatives for physical reservoir computing

Konrad Szaciłowski (AGH Univ., Kraków, Poland)

10:45 MS11_03

Streaming crystallography and Landau theory on the study of the out-of-equilibrium photo-induced phase transition in a RbMnFe Prussian Blue analogue

Ricardo Guillermo Torres Ramírez (Univ. Rennes, France)

11:05: MS11_04

Stacking interactions in “layered” energetic crystals: insights into electronic properties of supramolecular architecture defining macroscopic mechanical features

Iryna Omelchenko (ISN-NASU, Kharkiv, Ukraine)

11:25 MS11_05

Photomechanical motions in organoboron crystals featuring topochemical reactivity and phosphorescence emission

Subhrajyoti Bhandary (Ghent Univ., Belgium)

9:45: MS17 – Crystallographic methods to rescue natural and cultural heritage (1.B)

Chairs: Klaudia Hradil (TU Vienna, Austria), Alicja Rafalska-Łasocha (Jagiellonian Univ., Kraków, Poland)

9:45 MS17_01 / invited speaker

Imaging of alteration and degradation processes in 13th-20th c. works of art by MA-XRPD and related methods

Koen Janssens (Univ. Antwerp, Belgium)

10:15 MS17_02 / invited speaker

Geoscience for cultural heritage: challenges and innovative methods

Simona Raneri (Univ. Florence, Italy)

10:45 MS17_03

Betatron radiation compact sources: Tapping opportunities in cultural heritage and life sciences

Mattia Gaboardi (Univ. Rome Tor Vergata, Italy)

11:15 MS17_04

Terpene based co-crystals for the protection from biodeteriogens in archives and libraries

Andrea Ienco (ICCOM-CNR, Sesto Fiorentino, Italy)

9:45 MS27 – Insight into the crystal: crystal forms, isostructurality, symmetry, chirality (1.C)

Chairs: Petra Bombicz (TTK-MTA, Budapest, Hungary), Leopoldo Suescun (Univ. Republica, Montevideo, Uruguay)

9:45 MS27_01 / invited speaker

Informatics meets energetics: combining crystal structure prediction and knowledge of the crystal landscape

Emma Hawking (CCDC, Cambridge, United Kingdom)

10:15 MS27_02 / invited speaker

Probing the properties of perovskites by high pressure

Szymon Sobczak (Adam Mickiewicz Univ., Poznań, Poland)

10:45 MS27_03

Structural characterization and colour of $\text{CaMg}_{0.5}\text{Co}_x\text{Ni}_{0.5-x}\text{P}_2\text{O}_7$ ($0.0 \leq x \leq 0.5$) composition

Maria Angeles Tena (CINN-CSIC, Oviedo, Spain)

11:05 MS27_04

Chiral symmetry breaking in molecular crystals: emergence of isostructurality and tailored chirality

Anmol Andotra (Univ. Libre Brussels, Belgium)

11:25 MS27_05

Algorithms of symmetry measurement

Gil Alon (Open Univ. Israel, Haifa, Israel)

9:45 MS35 – Challenges of light sources, neutrons and XFEL (1.D)

Chair: Alke Meents (DESY, Hamburg, Germany)

9:45 MS35_03 / invited speaker

Using long-wavelength X-ray diffraction to localise light atoms in macromolecular crystals

Ramona Duman (Diamond LS, Didcot, United Kingdom)

10:15 MS35_02 / invited speaker

Many faces of SAXS – new SAXS beamline (SMAUG) for material science and biocrystallography in SOLARIS National Synchrotron Radiation Centre

Maciej Kozak (Adam Mickiewicz Univ., Poznań, Poland)

10:45 MS35_03

Neutron diffraction observed in the Earth's gravity field

Izabela Sosnowska (Univ. Warsaw, Poland)

11:05 MS35_04

MicroMAX – a beamline with time-resolved macromolecular crystallography capabilities at the MAX IV Laboratory

Dean Lang (MAX IV, Lund, Sweden)

11:25 MS35_05

Challenges and solutions for MX at beamline P11 on PETRA III

Johanna Hakanpää (DESY, Hamburg, Germany)

9:45 MS42 – Quantum mechanics and computational chemistry-based methods of crystallography (1.F)

Chairs: Anna Hoser (Univ. Warsaw, Poland), Horst Puschmann (Durham Univ., United Kingdom)

9:45 MS42_01 / invited speaker

GruPol: A database-driven framework for predicting biomolecular electrostatic and optoelectronic properties

Anna Krawczuk (Univ. Göttingen, Germany)

10:15 MS42_02 / invited speaker

Quantum crystallographic refinements from Machine Learning – Performance and speed benchmarks

Florian Kleemiss (RWTH-Aachen, Germany)

10:45 MS42_03

Program for automatic checking of crystal structure solution results based on comparison with DFT calculation results

František Fňukal (Univ. Chemistry & Technology, Prague, Czech Republic)

11:05 MS42_04

DiSCaMB – a package for exploring quantum crystallography

Michał Chodkiewicz (Univ. Warsaw, Poland)

11:25 MS42_05

Convergence study of a gradient-descent algorithm for Bloch amplitude refinement under the kinematical approximation

Kostas Bethanis (Agricultural Univ. Athens, Greece)

14:00 MS4 – Infectious and neglected diseases (1.E)

Chairs: Nicholas Furnham (LSHTM, London, UK), Matthias Wilmanns (EMBL Hamburg, Germany)

14:00 MS4_01 / invited speaker

Structural insights into the bacterial antiviral defense system Thoreris

Giedrė Tamulaitienė (Vilnius Univ., Lithuania)

14:30 MS4_02 / invited speaker

Accelerating antiviral drug discovery through high-throughput crystallographic fragment screening and structural enablement

Daren Fearon (Diamond LS, Didcot, United Kingdom)

15:00 MS4_03

Integrative, multi-temperature, time-resolved crystallography provides insight into molecular kinetics and dynamics of the Class A β -lactamase hydrolysis mechanism

Andreas Prester (UKE, Hamburg, Germany)

15:20 MS4_04

Targeting the Shigella-specific chaperone IpgC in drug development

Andreas Heine (Univ. Marburg, Germany)

15:40 MS4_05

Crystallographic structures of bacteriophage receptor-binding proteins and endolysins

Mark Van Raaij (CNB-CSIC, Madrid, Spain)

14:00 MS12 – Materials for energy storage and conversion (1.G)

Chairs: Laure Monconduit (Univ. Montpellier, France), Ihor Zavalii (PMINASU, Ukraine)

14:00 MS12_01 / invited speaker

How exotic synthesis path coupled with semi-automated processes can accelerate the discovery of new materials?

Gaël Minart (CIC energiGUNE, Minano, Spain)

14:30 MS12_02 / invited speaker

Metal hydrides for energy storage and hydrogenation reactions

Valérie Paul-Boncour (ICMPE, Paris, France)

15:00 MS12_03

Metal hydridoborates, novel materials for energy conversion and storage

Radovan Černý (Univ. Geneva, Switzerland)

15:20 MS12_04

Nowotny chimney-ladder phases

Kacper Pryga (AGH Univ., Kraków, Poland)

15:40 MS12_05

In-operando battery study of NMC811 and beyond: What a benchtop XRD can achieve

Simon Welzmler (Thermo Fisher Scientific, Ecublens, Switzerland)

14:00 MS20 – Aperiodic order and complex superstructures (1.B)

Chairs: Somnath Dey (FZU, Prague, Czech Republik), Julia Dshemuchadse (Cornell Univ., New York, USA), Eteri Svanidze (MPI Chemical Physics of Solids, Dresden, Germany)

14:00 MS20_01 / invited speaker

Aperiodic crystallography from 3-dimensional electron diffraction using kinematic and dynamical approaches

Gwladys Steciuk (Univ. Lorraine, Metz, France)

14:30 MS20_03

Structural chirality and functionality in incommensurate modulated tetragonal tungsten bronzes

Ola Grendal (NTNU, Trondheim, Norway)

14:50 MS20_04

Three refinement approaches to a description of a (3+1)D incommensurate modulated organic zwitterion dihydrate

Ilia Guzei (Univ. Wisconsin-Madison, USA)

15:10 MS20_02 / invited speaker

Aperiodic order and complex superstructures from simple algebraic rules

Wolfgang Hornfeck (FZU, Prague, Czech Republic)

15:40 MS20_05

Theoretical study of magnetism in Cd_6Tb 1/1 periodic cubic approximant of a Tsai-type quasicrystal

Gabriel Kuderowicz (AGH, Kraków, Poland)

14:00 MS28 – Molecular structure and chemical bonding (1.C)

Chairs: Teresa Duarte (Univ. Lisbon, Portugal), Christian Lehmann (MPI-Mülheim, Germany)

14:00 MS28_1 / invited speaker

From structure to reactivity: Quantum crystallography in organometallic chemistry

Florian Meurer (Univ. Regensburg, Germany)

14:30 MS28_2 / invited speaker

β -Turns, Peptides, Peptoids and CO $\cdots$ CO interactions

Consiglia Tedesco (Univ. Salerno, Italy)

15:00 MS28_3

Synthesis of heterometallic rare earth-zinc aryloxido complexes for catalytic applications

Adrian Kowaliński (Wrocław Univ. Science & Technology, Poland)

15:20 MS28_4

Linear dichroism and polarized photoluminescence in single crystals of Pt-containing NCN-pincer compound

Vitali Stsiapura (Univ. Warsaw, Poland)

15:40 MS28_5

Effect of phosphoryl group on a molecular structure: Rethinking resonance-assisted hydrogen bonds in P-containing systems

Anna Pietrzak (Lodz Univ. Technology, Poland)

14:00 MS36 – In situ and operando diffraction; time-resolved techniques (1.D)

Chairs: Mattia Gaboardi (Univ. Rome Tor Vergata, Italy), Bobby Joseph (Elettra, Trieste, Italy)

14:00 MS36_01 / invited speaker

Structural dynamics in Prussian Blue-based cathodes for ion batteries

Mariam Maisuradze (Univ. Bologna, Italy)

14:30 MS36_02 / invited speaker

Advancing crystallography with high-pressure single-crystal diffraction techniques

Umbertoluca Ranieri (MPC, San Sebastián, Spain)

15:00 MS36_03

Development of in situ X-ray diffraction techniques for characterization of stimuli-induced dynamics in MOFs

Volodymyr Bon (TU Dresden, Germany)

15:20 MS36_04

Three-faceted in situ setup for characterizing spinel high entropy oxides of 3d transition metal

Jens Edelvang-Pejrup (Univ. Copenhagen, Denmark)

15:40 MS36_05

Real-time observation of ultra-rapid densification and degradation in flash sintered monolithic all-solid-state batteries

Riku Fukuda (Institut Néel, Grenoble, France)

14:00 MS43 – Simulating and predicting structure (1.F)

Chairs: Lily Hunnisett (CCDC, Cambridge, United Kingdom), Jacco van de Streek (Avant-garde Materials Simulation, Merzhausen, Germany)

14:00 MS43_01 / invited speaker

Computational Organic Crystal Structure Prediction, an evolving challenge?

Sarah Price (Univ. College London, United Kingdom)

14:30 MS43_02 / invited speaker

Predicting crystal form stability under real-world conditions

Dzmitry Firaha (Avant-garde Materials Simulation, Merzhausen, Germany)

15:00 MS43_03

Exploring the crystal energy landscapes of polycyclic aromatic hydrocarbons via crystal structure prediction and Monte Carlo threshold algorithm

Pedro Juan Royo (Univ. Southampton, United Kingdom)

15:20 MS43_04

Investigating the role of solvents in metal-organic frameworks with molecular dynamic simulations

Yizhi Xu (Ruder Bošković Institute, Zagreb, Croatia)

15:40 MS43_05

Anharmonic effects in molecular crystals using quasiparticle theory

Ernesto Blancas (Univ. Oviedo, Spain)

16:30 - 17:15 Keynote lectures:

16:30 – 17:15 KEYNOTE 10 (1.E)

Toward understanding the molecular architecture of a glycogen-committed PP1/PTG holoenzyme: a putative target for Lafora disease

Paola Storici (Elettra, Trieste, Italy)

Chair: Sergi Plana-Ruiz (Univ. of Rovira i Virgili, Tarragona, Spain)

16:30 – 17:15 KEYNOTE 11 (1.G)

Crystals under pressure: their compression and intermolecular forces

Andrzej Katrusiak (Adam Mickiewicz Univ., Poznań, Poland)

Chair: Volodymyr Pavlyuk (Ivan Franko National Univ. of Lviv, Ukraine)

16:30 – 17:15 KEYNOTE 12 (1.B)

Synthase at the intersection of crystallography, energetics, and biophysical chemistry Chérif Matta (Mount Saint Vincent Univ., Halifax, Canada)

17:15 Kalman Prize (1.E)

Chair: Petra Bombicz (TTK-MTA, Budapest, Hungary)

From the Atom to the Framework: Crystallography at the Core of Reticular Chemistry

Felipe Gándara Barragán (Materials Science Institute of Madrid – CSIC, Spain)

Dr. Felipe Gándara Barragán has made significant contributions to the field of reticular chemistry over the last decade and has been deeply engaged in MOFs and COFs research. His innovative approach emphasizes the critical role of structural chemistry in understanding, controlling, and designing novel molecular-based materials with tailored properties for vital applications in energy and sustainability. He has pioneered crystallographic studies using a combination of experimental and computational techniques. Dr Gándara has made significant contributions to the education and dissemination of structural chemistry.

20:00 Conference dinner



**The Programme Committee and the Organizing Committee
of the 35th European Crystallographic Meeting**

have the honour to invite you to the

Conference dinner

which will take place on Wednesday, 27 August, at 20:00,

in the Earth Hall of the Poznań Conference Center,

10 Głogowska Street, Poznań.

Thursday, August 28

8:30 – 9:15 Keynote lectures:

8:30 – 9:15 KEYNOTE 13 (1.E)

Experimental charge density investigations: Data and model quality

Regine Herbst-Irmer (Univ. Göttingen, Germany)

Chair: Maura Malinska (Univ. of Warsaw, Poland)

8:30 – 9:15 KEYNOTE 14 (1.G)

Breaking boundaries, creating connections: The Cambridge Structural Database at 60

Suzanna Ward (CCDC, Cambridge, United Kingdom)

Chair: Bill Clegg (Newcastle Univ., United Kingdom)

9:45 MS3 – Software developments in MX and Cryo-EM including AI / Machine Learning (1.E)

Chairs: Maria Fando (STFC-UKRI, Oxford, United Kingdom), Isabel Uson (IBMB-CSIC, Barcelona, Spain)

9:45 MS3_01 / invited speaker

Coot & Moorhen: Interactive model building, refinement, and validation

Lucrezia Catapano (MRC-LMB, Cambridge, United Kingdom)

10:15 MS3_02 / invited speaker

Current developments in protein flexibility prediction

Sergei Grudinin (Univ. Grenoble, France)

10:45 MS3_03

Dictionary-driven atom type recognition for aspherical electron density reconstruction in macromolecules with the MATTS Data Bank

Paulina Rybicka (Univ. Warsaw, Poland)

11:05 MS3_04

A deep learning-powered ChimeraX plugin for ligand identification in CryoEM

Dariusz Brzezinski (Poznań Univ. Technology, Poland)

11:25 MS3_05

Validation of 3D cryoEM single particle reconstruction correctness and handedness with Ewald's sphere correction

Zbyszek Otwinowski (UT Southwestern Medical Center, Dallas, USA)

9:45 MS13 – Intermetallic compounds and derivatives (1.G)

Chairs: Vitaliy Romaka (TU Dresden, Germany), Yaroslav Tokaychuk (Ivan Franko National Univ. Lviv, Ukraine)

9:45 MS13_01 / invited lecture

A long-lasting exploration journey through classic, new and rediscovered approaches for studying Mg-containing intermetallics

Serena De Negri (Univ. Genova, Italy)

10:15 MS13_02 / invited speaker

Structural insights into ternary intermetallic nickel tetrelides

Viktor Hlukhyy (Technical Univ. Munich, Germany)

10:45 MS13_03

Structural database of kagome intermetallics: topology + geometry approach

Nataliia Hulai (Univ. Liverpool, United Kingdom)

11:05 MS13_04

Synchrotron X-ray powder diffraction investigation of the crystal structure of

$\text{HoCo}_{12}\text{B}_{6-x}\text{C}_x$

Kinan Al-Namourah (Univ. Grenoble Alpes, France)

11:25 MS13_05

Representatives of the Nowotny chimney-ladder phases in the Mo-Ge system

Bohdan Korotoshyn (Ivan Franko National Univ. Lviv, Ukraine)

9:45 MS21 – Surfaces, interfaces and ultrathin films (1.B)

Chairs: Julian Ledieu (Univ. Lorraine, Nancy, France), Hem Raj Sharma (Univ. Liverpool, United Kingdom)

9:45 MS21_01 / invited speaker

Probing atomic-scale structures at electrochemical interfaces using in-situ X-ray diffraction

Yvonne Grunder (Univ. Liverpool, United Kingdom)

10:15 MS21_02

Towards quantitative evaluation of grazing incidence X-ray diffraction data

Fabian Gasser (Graz Univ. Technology, Austria)

10:35 MS21_03

XRD study of thin films of Y-type hexaferrites prepared by chemical solution deposition

Radomír Kužel (Charles Univ., Prague, Czech Republic)

10:55 MS21_04 / invited speaker

Structure determination by low-energy electron diffraction – A roadmap to the future

Georg Held (Diamond LS, Didcot, United Kingdom)

11:25 MS21_05

Application and challenge on characterization of thin-crystalline organic material structures with electron diffraction

Kiyofumi Takaba (Univ. Vienna, Austria)

9:45 MS29 – Impact of non-covalent interactions on dynamics in molecular crystals (1.C)

Chairs: Amy Hall (Durham Univ., United Kingdom), Izabela Madura (Warsaw Univ. Technology, Poland)

9:45 MS29_01 / invited speaker

Impact of coformer substitution on the formation and polymorphism of pharmaceutical cocrystals

Doris Brown (Univ. Innsbruck, Austria)

10:15 MS29_02 / invited speaker

Spatial and temporal visualization of polymorphic transformations in pharmaceutical tablets

Iain Oswald (Univ. Strathclyde, United Kingdom)

10:45 MS29_03

Influence of sulfur...oxygen, π ... π /C-H... π and other intermolecular interactions on molecular switching of the NO₂ ligand in polymorphic forms of a nickel(II) complex

Kinga Potempa (Univ. Warsaw, Poland)

11:05 MS29_04

Exploring non-covalent interactions in simple binary adducts by a combination of DSC and variable temperature powder and single-crystal X-ray diffraction

Jeremy Cockcroft (Univ. College London, United Kingdom)

11:25 MS29_05

Atomic-level mechanism underlying elastic flexibility of coordination polymer crystals

Marijana Đaković (Univ. Zagreb, Croatia)

9:45 MS37 – Advanced and new techniques to study inorganic materials (1.D)

Chairs: Mariana Klementova (FZU-CAS, Prague, Czech Republic), Andrew Stewart (Univ. College London, United Kingdom)

9:45 MS37_01 / invited speaker

Direct imaging of beam-sensitive inorganic materials using 2D and 4D scanning transmission electron micros

Peter Nellist (Oxford Univ., United Kingdom)

10:15 MS37_02 / invited speaker

Accessing the phonon dispersion of nanostructures via grazing incidence inelastic x-ray scattering spectroscopy

Daniel Chaney (ESRF, Grenoble, France)

10:45 MS37_03

Combined μ XRD and μ XRF mapping of hierarchical materials – atomic structure, crystallographic texture and chemical mapping over large areas

Mads Ry Vogel Jørgensen (Aarhus Univ., Denmark)

11:05 MS37_05

Structure of a DNA-stabilized $\text{Ag}_{16}\text{Cl}_2$ nanocluster in solution

Adam Sapnik (Univ. Copenhagen, Denmark)

11:25 MS37_06

Chemical bonding as structure and property directing motif in functional materials

Joachim Breternitz (FH Münster Univ. Applied Sciences, Germany)

9:45 MS44 – Comparing crystal structures in massive datasets (1.F)

Chairs: Nicholas Francia (CCDC, Cambridge, United Kingdom), Martin Lutz (Utrecht Univ., The Netherlands)

9:45 MS44_01 / invited speaker

Comparing crystal structures: isostructurality

Petra Bombicz (TTK-MTA, Budapest, Hungary)

10:15 MS44_02 / invited speaker

Quantitative crystal structure comparison using powder diffractograms

Erin Johnson (Dalhousie Univ., Halifax, Canada)

10:45 MS44_03

Powder-diffraction-based structural comparison for crystal structure prediction under pressure

Alberto Otero-de-la-Roza (Univ. Oviedo, Spain)

11:05 MS44_04

Are crystal structures getting better? A statistical analysis of the Cambridge Structural Database

Florian Meurer (Univ. Regensburg, Germany)

11:25 MS44_05

Growth functions of periodic space tessellations

Jakub Malinowski (Wroclaw Univ. Science & Technology, Poland)

14:00 MS6 – Fragment screening and structural based drug discovery (1.E)

Chairs: Daren Fearon (Diamond LS, Didcot, United Kingdom), Tobias Krojer (MAX IV, Lund, Sweden)

14:00 MS6_01 / invited speaker

Structure-based hit discovery for protein and RNA targets for antibiotics

Ruth Brenk (Univ. Bergen, Norway)

14:30 MS6_02 / invited speaker

Preserving and publishing crystallographic fragment-screening data

Manfred Weiss (Helmholtz-Zentrum Berlin, Germany)

15:00 MS6_03

High-throughput fixed target SFX for pharmaceutical screening at the European XFEL

Peter Smyth (European XFEL, Schenefeld, Germany)

15:20 MS6_04

New horizons for structure-based discovery of PYCR1 inhibitors

Milosz Ruszkowski (IBCH-PAN, Poznań, Poland)

15:40 MS6_05

Covalent fragment-based drug discovery as a strategy to combat leishmaniasis

Maria Cristina Nonato (Univ. Sao Paulo, Brazil)

14:00 MS14 – From crystal structure to magnetic structure (1.G)

Chairs: Françoise Damay (LLB-CEA, Paris, France), Khrystyna Miliyanchuk (Ivan Franko National Univ., Lviv, Ukraine)

14:00 MS14_01 / invited speaker

Magnetic modulations in bulk α -BiFeO₃ described using monoclinic superspace groups

Izabela Sosnowska (Univ. Warsaw, Poland)

14:30 MS14_02 / invited speaker

Crystal symmetry and magnetic structures in frustrated and non-frustrated Ho systems

Margarida Henriques (FZU, Prague, Czech Republik)

15:00 MS14_03

Complex magnetic properties of RE₅T₂In₄ (RE = Gd-Tm; T = Ni, Rh, Pd, Pt) intermetallics

Stanisław Baran (Jagiellonian Univ., Kraków, Poland)

15:20 MS14_04

Study of the magnetic structure of the helimagnet YBaCuFeO₅ using neutron and x-ray scattering

Chao-hung Du (Tamkang Univ., New Taipei City, Taiwan)

15:40 MS14_05

Magnetic anisotropy in layered vanadyl phosphates: Insights from DFT+U and X-ray charge density studies

Lovro Saric (Univ. Bern, Switzerland)

14:00 MS19 – Quantum mechanical models for disorder, dynamics, and diffuse scattering (1.B)

Chairs: Johnathan Bulled (ESRF, Grenoble, France), Anders Østergaard Madsen (Univ. Copenhagen, Denmark)

14:00 MS19_01 / invited speaker

Combining single crystal diffuse scattering and ab initio molecular dynamics simulations to understand framework dynamics in AlPO_4 -5

Ella Schmidt (Univ. Bremen, Germany)

14:30 MS19_02 / invited speaker

Local structure studies using neutrons and X-rays augmented with theory

Matthias Gutmann (ISIS Facility, Didcot, United Kingdom)

15:00 MS19_03

Local structure and dynamics in $\text{MPt}(\text{CN})_6$ Prussian Blue analogues

Elodie Harbourne (Univ. Oxford, United Kingdom)

15:20 MS19_04

“Correlated disorder” is not disorder and can change lattice energies by >2.5 kcal/mol

Jacco Van de Streek (Avant-garde Materials Simulation, Merzhausen, Germany)

15:40 MS19_05

Direct derivation of the atomic displacement parameters with molecular dynamics simulations

Yoyo Hinuma (AIST, Osaka, Japan)

14:00 MS30 – Polymorphism and phase transitions (1.C)

Chairs: Alessia Bacchi (Univ. Parma, Italy), Szymon Sobczak (Adam Mickiewicz Univ., Poznań, Poland)

14:00 MS30_01 / invited speaker

Experimentally exploring the polymorphism of ROY through high throughput crystallization

Michael Probert (Newcastle Univ., United Kingdom)

14:30 MS30_02 / invited speaker

Discovery of new polymorphs of metal organic frameworks via mechanochemical screening

Ivana Brekalo (Ruder Boskovic Institute, Zagreb, Croatia)

15:00 MS30_03

Triethylphosphine: a ‘molecular gear’ enabling single-crystal-to-single-crystal phase transitions

Anna Makal (Univ. Warsaw, Poland)

15:20 MS30_03

Fascinating polymorphism in Lapachol powders

Leopoldo Suescun (Univ. Republica, Montevideo, Uruguay)

15:40 MS30_04

Three new polymorphs of glyphosate under extreme conditions

Chengdao Hu (Univ. Edinburgh, United Kingdom)

14:00 MS38 – Powder diffraction on organic compounds (1.D)

Chairs: Federica Bravetti (Univ. Frankfurt, Germany), Maria Spiliopoulou (UKE, Hamburg, Germany)

14:00 MS38_01 / invited speaker

Advancing structure solution of organic compounds: Strategies for tackling XRPD challenges

Angela Altomare (IC-CNR, Bari, Italy)

14:30 MS38_02 / invited speaker

Exploring high-throughput synchrotron X-ray powder diffraction for the characterization of pharmaceuticals

Mathilde Reinle-Schmitt (Excelsul Strutural Solutions (Swiss) AG, Switzerland)

15:00 MS38_03

Solving structures from powders using intermolecular distances

Jan Rohlicek (FZU-CAS, Prague, Czech Republic)

15:20 MS38_04

Complementarity of PXRD and ssNMR in structure solution of meloxicam multicomponent crystals

Przemysław Nowak (Univ. Lodz, Poland)

15:40 MS38_05

Matching powder patterns to crystal structures with AutoFIDEL

Andrew Maloney (CCDC, Cambridge, United Kingdom)

14:00 MS45 – How to... successfully apply for funding (1.F)

Chairs: Santiago Garcia-Granda (CINN-CSIC, Oviedo, Spain), Matic Lozinšek (JSI, Ljubliana, Slovenia), Marta Morana (Univ. Florence, Italy)

14:00 MS45_01 / invited speaker

Trying, failing, and sometimes succeeding: One researcher's journey through funding applications

Anna Krawczuk (Univ. Göttingen, Germany)

14:30 MS45_02 / invited speaker

Drafting a successful proposal for state-of-the-art experiments at large-scale and medium-range research infrastructures

Mattia Gaboardi (Univ. Rome Tor Vergata, Italy)

15:00 MS45_03

How to... find your niche in a few steps

Kamil Dziubek (Univ. Vienna, Austria)

15:20 MS45_04

GEMS: revealing the hidden treasure of the European crystallographic community

Mateja Pisačić (Univ. Zagreb, Croatia)

15:40 Open discussion

16:30 – 17:15 Keynote lectures:

16:30 – 17:15 KEYNOTE 15 (1.E)

Complementing powder diffraction with inelastic information – iron oxide nanoparticles as an example

Mirijam Zobel (RWTH-Aachen, Germany)

Chair: Klaudia Hradil (Vienna Univ. of Technology, Austria)

16:30 – 17:15 KEYNOTE 16 (1.G)

Journey into the fascinating world of aperiodic crystals

Marc de Boissieu (Univ. Grenoble Alpes, France)

16:30 – 17:15 KEYNOTE 17 (1.B)

Crystallography beyond Independent Atom Model

Krzysztof Woźniak (Univ. Warsaw, Poland)

17:15 Science slam (1.E)

SCIENCE SLAM



**AUGUST 28
AT 17:15**

Lights, lab coats, action!



What is Slam

A fun, fast-paced science showdown, where researchers present their favourite crystallographic topic in an exciting and understandable way.

How it works

- 5 minutes on stage
- any form goes: slides, props, dance or song
- be clear, creative, and captivating

Prizes

Fame! Glory! And awesome prizes for the top 3 performers, chosen by the audience.

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Send an email on scienceslam.ecm@gmail.com with your name, affiliation, and short abstract.

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AUGUST 2025



SINCE 1887

19:00 Open lecture

III Liceum Ogólnokształcące im. św. Jana Kantego, Strzelecka 10, Poznań



The Programme Committee and the Organizing Committee of the 35th European Crystallographic Meeting

have the honour to invite you to the

Open lecture

The Nobel winner Max von Laue was a schoolboy in Poznań

which will be delivered by Prof. Andrzej B. Więckowski

on Thursday, 28 August, at 19:00,

at III Liceum Ogólnokształcące im. Św. Jana Kantego,

10 Strzelecka Street, Poznań.

Andrzej B. Więckowski (Poznań, Zielona Góra)

The Nobel winner Max von Laue was a schoolboy in Poznań

Max Theodor Felix von Laue (1879-1960) was one of the greatest physicists of the 20th century. He was born on 9th October, 1879. The ideas of Max von Laue on the interaction of X-rays with atoms led to the discovery of X-ray interferences on crystals in radiographs which, following his initiative, were made by Walter Friedrich (1883-1968) and Paul Knipping (1883-1935) in the University of Munich in the year 1912. On the basis of his courageous explanation of the diffraction phenomenon of X-rays on crystals, he received the Nobel Prize in physics for the year 1914. With this discovery Max von Laue confirmed the wave nature of X-rays and the three-dimensional lattice structure of crystals as well. Max von Laue died after a car accident on 24th April, 1960.

Till 1996, we knew very little about the time of the childhood of Max von Laue spent in Poznań. My purpose to follow the traces of a pupil living in the 19th century in the former province metropolis of Poznań was from the practical point of view a hopeless undertaking, and it seemed that this venture would encounter big difficulties. Unknown were the answers to the questions, when the Laue family came to Poznań, where they were living, or which school the young Max Laue attended. Gradually, I have found some answers to these questions. Additionally, I got more precise indications about the birthplace of Max Laue. According to the documents kept in the State Archive in Poznań, it is most likely that Max Laue was born in the suburb Pfaffendorf (registry Ehrenbreitstein) near Coblenz.

The documents mentioned above include the registration card of the Laue family upon their arrival in Poznań, and the entry in the directory of pupils of the Royal Friedrich-Wilhelms-Gymnasium in Poznań (*Königliches Friedrich-Wilhelms-Gymnasium zu Posen*). Also, 13 school certificates of the pupil Max Laue from the years 1887-1891 were found. As a schoolboy, Max Laue was a young urchin, with appropriate notes in his certificates. We can also learn that he had mostly satisfactory school grades. His grade for nature lessons was “good” in 1888 and “very good” in 1891.

In 2014, on the occasion of the International Year of Crystallography, a commemorative plaque in honor of Max von Laue was unveiled on the façade of the his school building, which is now the 3rd St. John Cantius Lycée in Poznań.

Professor Andrzej B. Więckowski is a physicist and chemist, specializing in the history of physics. He will present his research on Max von Laue’s school years in Poznań, revealing documents confirming Laue’s education at the Friedrich-Wilhelms-Gymnasium. The lecture will also describe von Laue’s Nobel Prize-winning discovery. In 2014, a plaque was unveiled at von Laue’s school, to mark the International Year of Crystallography and to highlight Laue’s connection to Poznań. The lecture will take place in the very school attended by Max von Laue.

Friday, August 29

8:30 – 9:15 Keynote lectures:

8:30 – 9:15 KEYNOTE 18 (1.E)

Bridging the gap. Serial crystallography at 4th generation synchrotrons: Current status and future goals

Daniele de Sanctis (ESRF, Grenoble, France)

Chair: Michele Cianci (Polytechnic Univ. of Marches, Ancona, Italy)

8:30 – 9:15 KEYNOTE 19 (1.G)

Single crystals and beyond – research and study in Kharkiv amid explosions and air alarms

Ilias Shcherbakov (ISC-NASU, Kharkiv, Ukraine)

Chair: Kamil Dziubek (Univ. of Vienna, Austria)

9:45 MS7 – Electron diffraction of macromolecules (1.E)

Chairs: David Owen (Diamond LS, Didcot, United Kingdom), Xiaodong Zou (Stockholm Univ., Sweden)

9:45 MS7_01 / invited speaker

Counting and filtering macromolecular electron diffraction data

Max Clabbers (Aarhus Univ., Denmark)

10:15 MS7_02 / invited speaker

Developing electron diffraction methods to probe oxidation states in metalloenzymes

Laura Pacoste (Stockholm Univ., Sweden)

10:45 MS7_03

Modelling the protein electrostatic potential Fourier maps across resolutions

Marta Kulik (Univ. Warsaw, Poland)

11:05 MS7_04

HeXI: The High-energy Electron Xtallography Instrument

Alistair Siebert (Diamond LS, Didcot, United Kingdom)

11:25 MS7_05

Adapting the YoneoLocr package for automated data processing at the Electron Bio-Imaging Centre

Marko Petrovic (STFC Rutherford Appleton Lab., Didcot, United Kingdom)

9:45 MS15 – Inorganic crystal structure investigation using electron diffraction (1.G)

Chairs: Stéphanie Kodjikian (Institut Néel, Grenoble, France), Louisa Meshi (Ben-Gurion Univ. Negev, Beersheba, Israel)

9:45 MS15_01 / invited speaker

Scanning electron crystallography powered by machine learning

Yevgeny Rakita (Ben-Gurion Univ. Negev, Beersheba, Israel)

10:15 MS15_02 / invited speaker

Advanced electron diffraction techniques for functional material structural analysis

Christophe Lepoittevin (Institut Néel, Grenoble, France)

10:45 MS15_03

Revealing invisibles: Analysis of complex structures by 3D electron diffraction

Zhehao Huang (Stockholm Univ., Sweden)

11:05 MS15_04

Direct quantitative and localisation of aluminum in individual zeolite crystals by 3D Electron Diffraction

Soheil Mahmoudi (Univ. Vienna, Austria)

11:25 MS15_05

Rapid development of a vast family of MOFs facilitated by 3D electron diffraction

Andrew Kentaro Inge (Stockholm Univ., Sweden)

9:45 MS23 – Dynamics and disorder in complex systems and/or under extreme conditions (1.B)

Chairs: Daniel Chaney (ESRF, Grenoble, France), Ella Schmidt (Univ. Bremen, Germany)

9:45 MS23_01 / invited speaker

X-ray diffuse scattering at high pressures

Björn Wehinger (ESRF, Grenoble, France)

10:15 MS23_02 / invited speaker

Resolving fast relative kinetics of inorganic materials from in situ studies

Bryce Mullens (Stoney Brook Univ., New York, USA)

10:45 MS23_03

High pressure phase transition in groutite, $\text{MnO}(\text{OH})$

Roman Gajda (Univ. Warsaw, Poland)

11:05 MS23_04

Uncovering stacking disorder in the Weyl semimetal TaRhTe_4

Felix Eder (Univ. Geneva, Switzerland)

11:25 MS23_05

Exploring structural disorder in natural and synthetic pyrochlores through single crystal X-ray diffuse scattering

Giovanni Orazio Lepore (Univ. Florence, Italy)

9:45 MS31 – Crystallography in the world of mechanochemistry (1.C)

Chairs: Dritan Hasa (Univ. Trieste, Italy), Adam Michalchuk (Univ. Birmingham, United Kingdom)

9:45 MS31_01 / invited speaker

Mechanochemical reactivity of halogen-bonded materials: computational prediction of reaction outcome and spectroscopic monitoring

Mihails Arhangel'skis (Univ. Warsaw, Poland)

10:15 MS31_02 / invited speaker

Pushing the limits: Evolving twin-screw extrus

Deborah Crawford (Univ. Birmingham, United Kingdom)

10:45 MS31_03

Potential of mechanochemistry in the preparation of novel multicomponent supramolecular systems containing praziquantel

Mateusz Gołdyn (Adam Mickiewicz Univ., Poznań, Poland)

11:05 MS31_04

Analysis of individual nanocrystals in phase mixtures by 3D electron diffraction

Christian Jandl (ELDICO Scientific AG, Allschwil, Switzerland)

11:25 MS31_05

Co-crystals on stage: Time resolved in situ monitoring of multicomponent mechanochemical reactions

Alessia Bacchi (Univ. Parma, Italy)

9:45 MS39 – High-pressure crystallography (1.D)

Chairs: Anna Makal (Univ. Warsaw, Poland), Andrzej Katrusiak (Adam Mickiewicz Univ., Poznań, Poland)

9:45 MS39_01 / invited speaker

High-pressure synthesis and diffraction studies on functional materials using in situ X-ray and neutron diffraction

Karen Friese (Forschungszentrum Jülich, Germany)

10:15 MS39_02 / invited speaker

Hydrogen storage in hydrogen hydrates at high pressure

Tomasz Poręba (EPFL, Lausanne, Switzerland)

10:45 MS39_03

Compressing secondary arsenic...halogen bonds: high-pressure X-ray diffraction study of As₂O₃ intercalation compounds

Piotr Guńka (Warsaw Univ. Technology, Poland)

11:00 MS39_04

High-pressure study of the charge density wave evolution in SmNiC₂

Andreas Eich (KIT, Karlsruhe, Germany)

11:15 MS39_05

Symmetrization of strong hydrogen bond under high pressure in bihydroxide-ion-containing NaCu₂(SO₄)₂·H₃O₂ revealed by experimental charge density and single crystal electron and neutron diffraction study

Piotr Rejnhardt (Univ. Warsaw, Poland)

11:30 MS39_06

Giant piezochromic shift in square planar Rh(I) complexes: Reversible red-to-NIR optical switching under pressure

Vishnu Vijayakumar Syamala (Univ. Warsaw, Poland)

9:45 MS47 – Exploiting crystallographic databases in solving, refining, and validating crystal structures (1.F)

Chairs: Michael Probert (Newcastle Univ., United Kingdom), Suzanna Ward (CCDC, Cambridge, United Kingdom)

9:45 MS47_01 / invited speaker

Back to (data) basics – How crystallographic databases can help solve new structures

Natalie Johnson (CCDC, Cambridge, United Kingdom)

10:15 MS47_02 / invited speaker

Jumping the hurdles: Challenges in calculating thermal expansion coefficients from the data in the Cambridge Structural Database

Arie van der Lee (Univ. Montpellier, France)

10:45 MS47_03

Hands-on learning activities for chemical crystallography students derived from data and tools provided by the Cambridge Crystallographic Data Centre

Diane Dickie (Univ. Virginia, Charlottesville, USA)

11:05 MS47_04

Rigid groups, model restraints, elusive H atoms... practical examples of using CSD entries to help with difficult structures

William Clegg (Newcastle Univ., United Kingdom)

11:25 MS47_05

Towards a double verified (experimental + DFT) reference structure database

Michal Hušák (Univ. Chemistry & Technology, Prague, Czech Republic)

14:00 MS8 – Cross-method structural studies (1.E)

Chairs: Eilis Bragginton (Diamond LS, Didcot, United Kingdom), Giorgia Fiorini (PSI Villigen, Switzerland)

14:00 MS8_01 / invited speaker

From colour change to pathology: Mechanisms of crystal formation and morphogenesis in pigment cells

Dvir Gur (Weizmann Institute of Science, Rehovot, Israel)

14:30 MS8_02 / invited speaker

Following antibiotic degradation by a β -lactamase using room-temperature crystallography and biomolecular simulation

Catherine Tooke (Univ. Bath, United Kingdom)

14:50 MS8_03

X-ray based multi-modalities to understand complex (nano)material systems with applications in biomedicine

Antonia Neels (EMPA, Dübendorf, Switzerland)

15:10 MS8_04

Anomalous crystallography – Can we see oxidation states in crystal structures?

Michael Bodensteiner (Univ. Regensburg, Germany)

15:30 MS8_05

Cryo-EM structure of *Homarus americanus* α -crustacyanin reveals the astaxanthin molecular tuning in marine invertebrate colouration

Michele Cianci (Univ. Politecnica delle Marche, Ancona, Italy)

14:00 MS16 – Crystallography of minerals in the Universe (1.G)

Chairs: Tiziana Boffa-Ballaran (Univ. Bayreuth, Germany), Przemyslaw Dera (Univ. Hawaii, Honolulu, USA)

14:00 MS16_01 / invited speaker

When crystallography meets planetary science: Insights into large icy moons of Jupiter and Saturn

Anna Pakhomova (ESRF, Grenoble, France)

14:30 MS16_02

Minerals on Titan: The crystal structure of diacetylene

Larissa Lopes Cavalcante (Univ. Otago, Dunedin, New Zealand)

14:50 MS16_03

A new terrestrial Ti^{3+} -rich oxide with a novel crystal structure

Marcin Stachowicz (Univ. Warsaw, Poland)

15:10 MS16_04

Structure of ferrosilite and pentlandite from inclusions in the Muong Nong tektites from Laos

Mariana Klementová (FZU-CAS, Prague, Czech Republic)

15:30 MS16_05

A new kristiansenite-like mineral from post-magmatic mineralization in the Szklarska Poręba granite?

Sylwia Zelek-Pogudz (AGH Univ., Kraków, Poland)

14:00 MS24 – Disordered and defective molecular systems, effect on chemical properties (1.B)

Chairs: Hanna Boström (Stockholm Univ., Sweden), Stefano Canossa (ETH Zurich, Switzerland)

14:00 MS24_01 / invited speaker

Tuning the local structure of isorecticular porous materials

Emily Meekel (Kyoto Univ., Japan)

14:30 MS24_02 / invited speaker

Nanocrystalline organic compounds: structure determination by a global fit to the pair-distribution function

Martin Schmidt (Frankfurt Univ., Germany)

15:00 MS24_03

The polymorph myth dispelled: True forms of oxytetracycline hydrochloride

Martyna Pęczek (Univ. Warsaw, Poland)

15:15 MS24_04

Searching for the hidden phases of Fe(II) metal-organic SCO frameworks

Elzbieta Trzop (Univ. Rennes, France)

15:30 MS24_05

Hydrogenation–disordering of structure” correlations for Ni/Co-based nanomaterial

Ihor Zavaliy (Physico-Mechanical Institute NASU, Lviv, Ukraine)

15:45 MS24_06

Controlling the superionic transition temperature through anion substitution in CuCrX₂ (X = S, Se, Te)

Alexandra Zevalkink (Michigan State Univ., East Lansing, USA)

14:00 MS26 – The complex world of multicomponent crystals (1.C)

Chairs: Consiglia Tedesco (Univ. Salerno, Italy), Kateryna Terebilenko (Kyiv National Univ., Ukraine)

14:00 MS26_01 / invited speaker

Calixarene-based multicomponent crystals: solvent selectivity, conformational dynamics, and supramolecular assembly

Maura Malinska (Univ. Warsaw, Poland)

14:30 MS26_02 / invited speaker

Harnessing the structural diversity of multicomponent crystals: strategies from synthesis to functional properties

Mattia Lopresti (Univ. Eastern Piedmont, Alessandria, Italy)

15:00 MS26_03

Trimesic acid as a highly efficient scaffold for trapping essential oil terpenoids

Andrea Daolio (Univ. Parma, Italy)

15:15 MS26_04

Al-Fe B2 as a model for studying defects and long-range order in the AlCoCrFeNi multicomponent system

Louisa Meshi (Ben Gurion Univ. Negev, Beer-Sheva, Israel)

15:30 MS26_05

The potential of microwaves and mechanochemistry in obtaining novel multicomponent forms of theophylline with benzene-1,2,4,5-tetracarboxylic acid as a conformer

Elżbieta Bartoszak-Adamska (Adam Mickiewicz Univ, Poznań, Poland)

15:45 MS26_06

Design and characterization of multicomponent forms of miconazole: structural, biological, and solubility studies

Anna Ben (Univ. Lodz, Poland)

14:00 MS40 – New developments in electron diffraction (1.D)

Chairs: Paul Klar (Univ. Bremen, Germany), Ute Kolb (Univ. Mainz, Germany)

14:00 MS40_01 / invited speaker

Experimental charge densities of organic nanocrystals from 3D electron diffraction

Paulina Dominiak (Univ. Warsaw, Poland)

14:30 MS40_02 / invited speaker

Crystal structure determination and refinement from serial precession electron diffraction

Sergi Plana-Ruiz (Univ. Rovira i Virgili, Tarragona, Spain)

15:00 MS40_03

Reporting 3D ED structures made easier: The changes in the core CIF dictionary to allow consistent, correct, and complete reporting of 3D ED structure refinements

Lukas Palatinus (FZU-CAS, Prague, Czech Republic)

15:20 MS40_04

Reproducible electron diffraction simulations: Bridging Bloch wave and multislice simulations with abTEM

Małgorzata Cabaj (FZU-CAS, Prague, Czech Republic)

15:40 MS40_05

Characterising particle-to-crystal transitions: Analytical approaches and implications for 3DED

Andrew Stewart (Univ. College London, United Kingdom)

14:00 MS46 – Publishing crystallography (1.F)

Chairs: William Clegg (Newcastle Univ., United Kingdom), Chiara Massera (Univ. Parma, Italy)

14:00 MS46_01 / invited speaker

How do I publish my paper?

Louise Jones (IUCr, Chester, United Kingdom)

14:30 MS46_02 / invited speaker

Ethical publishing of crystallographic papers

Manfred Weiss (Helmholtz-Zentrum Berlin, Germany)

15:00 MS46_03

Tackling the challenge of unpublished structures

Gary Nichol (Univ. Edinburgh, United Kingdom)

15:20 MS46_04

Raw data and external links in the Crystallography Open Database

Saulius Gražulis (Vilnius Univ., Lithuania)

15:40

Publishing crystallography in the 21st century

open discussion led by William Clegg

Plenary lecture 2 (1.E)

16:30 – 17:15 Plenary lecture 2

Chair: Maciej Kubicki (Adam Mickiewicz Univ., Poznań, Poland)

AI/ML in crystallography: What can it do for us, what can we do with it?

Simon Billinge (Columbia Univ., New York, USA)

17:15 Closing ceremony (1.E)

Poster prizes (Grygoriy Dmytriv)

Arie van der Lee, ECA President

Roman Gladyshevskii, Chair of the Program Committee ECM35

Maciej Kubicki, Chair of the Organizing Committee ECM35

Radomir Kuzel Chair of Organising Committee ECM36