Monday, August 25

17:00 Opening ceremony

Ambassador of Ukraine to Poland – Vasyl Bodnar

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)

8:30 – 9:15 KEYNOTE 2 (1.A)

Crystallochemistry underneath function: in situ power diffraction at work
Simona Galli (Univ. Insubria, Como, Italy)

8:30 – 9:15 KEYNOTE 3 (1.B)

George Sheldrick's SHELX: success for all
Isabel Uson (IMB Barcelona, Spain)

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.A)

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 conkit-validate
Adam Simpkin (Univ. Liverpool, United Kingdom)

10:15 MS9_02 / invited speaker
Validation of symmetric protein assemblies predicted by SymProFold
Christoph Grininger (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
Przemyslaw Rzepka (CAS, Prague, Czech Republic)

10.45 MS22_03
Lack of long-range order in 'relaxor' ferroelectric $NH_4Zn(HCOO)_3$: 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 $Ce_{0.5}Ba_{0.5}MnO_3$ 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
Gold supramolecular chemistry beyond aurophilic phenomena: New and less known interactions
Emanuele Priola (Univ. Turin, Italy)

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
Back to morphology: streamlined modelling of crystals' growth from solutions
Yevhenii Vaksler (Janssen R&D, Beerse, Belgium)

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-ΔPDF 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 sructural dynamics of cytochrome c oxydase
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.A)

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 $Cu_6Te_{3-x}S_{1+x}$: 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)

16:30 – 17:15 KEYNOTE 5 (1.A)

Electron density and chemical bonding in intermetallic compounds
Juri Grin (MPI Chemical Physics of Solids, Dresden, Germany)

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)

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)

8:30 – 9:15 KEYNOTE 8 (1.A)

A Journey to the Nanoscale through Electron Diffraction
Sergi Plana Ruiz (Univ. Rovira i Virgili, Tarragona, Spain)

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)

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.A)

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 Ranieri (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 $CaMg_{0.5}Co_xNi_{0.5-x}P_2O_7$ ($0.0 \leq x \leq 0.5$) 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 (LSHTHM, London, UK), Matthias Wilmanns (EMBL Hamburg, Germany)

14:00 MS4_01 / invited speaker
Structural insights into the bacterial antiviral defense system Thoeris
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.A)

Chairs: Laure Monconduit (Univ. Montpellier, France), Ihor Zavaliy (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 Welzmiller (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 · · · 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), Boby 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 (Ruđer 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)

16:30 – 17:15 KEYNOTE 11 (1.A)

Crystals under pressure: their compression and intermolecular forces
Andrzej Katrusiak (Adam Mickiewicz Univ., Poznań, Poland)

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)

8:30 – 9:15 KEYNOTE 14 (1.A)

Breaking boundaries, creating connections: The Cambridge Structural Database at 60
Suzanna Ward (CCDC, Cambridge, 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.A)

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 $HoCo_{12}B_{6-x}C_x$
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 NO_2 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 µXRD and µXRF 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 $Ag_{16}Cl_2$ 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.A)

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-$BiFeO_3$ 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 $RE_5T_2In_4$ (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 $YBaCuFeO_5$ 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 $MPt(CN)_6$ 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 (PSI Villigen, 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, Liubliana, 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)

16:30 – 17:15 KEYNOTE 16 (1.A)

Journey into the fascinating world of aperiodic crystals
Marc de Boissieu (Univ. Grenoble Alpes, France)

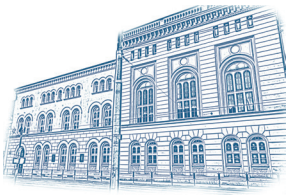
16:30 – 17:15 KEYNOTE 17 (1.B)

Crystallography beyond Independent Atom Model
Krzysztof Woźniak (Univ. Warsaw, Poland)

17:15 Science slam (1.E)

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)

8:30 – 9:15 KEYNOTE 19 (1.A)

Single crystals and beyond – research and study in Kharkiv amid explosions and air alarms
Ilias Shcherbakov (ISC-NASU, Kharkiv, Ukraine)

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.A)

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, MnO(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 Arhangelskis (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 As_2O_3 intercalation compounds
Piotr Guńka (Warsaw Univ. Technology, Poland)

11:00 MS39_04
High-pressure study of the charge density wave evolution in $SmNiC_2$
Andreas Eich (KIT, Karlsruhe, Germany)

11:15 MS39_05
Symmetrization of strong hydrogen bond under high pressure in bihydroxide-ion-containing $NaCu_2(SO_4)_2 \cdot H_3O_2$ 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 MS16_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 MS16_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 MS16_03
X-ray based multi-modalities to understand complex (nano)material systems with applications in biomedicine
Antonia Neels (EMPA, Dübendorf, Switzerland)

15:10 MS16_04
Anomalous crystallography – Can we see oxidation states in crystal structures?
Michael Bodensteiner (Univ. Regensburg, Germany)

15:30 MS16_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.A)

Chairs: Tiziana Boffa-Ballaran (Univ. Bayreuth, Germany), Przemyslav Dera (Univ. Hawai, 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 isoreticular 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 though 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