

SESJA PLENARNA 2 / PLENARY SESSION 2

Sesja specjalna dotycząca badań z użyciem XFEL Special session on research using XFEL

- 11:15 – 11:45** **Przemysław Nogły** **R-5**
Time-resolved X-ray crystallography on membrane proteins: watching ions moving in time and space
Jagiellonian University, Kraków
- 11:45 – 12:15** **Doriana Vinci**, Karl Ridier, Fengfeng Qi, Fernando Ardana Lamas, Peter Zalden, Lai Chun Liu, Tobias Eklund, Mads Sielemann Jakobsen, Robin Schubert, Dmitry Khakhulin, Carsten Deiter, Nicolas Bottin, Hazem Yousef, David von Stetten, Celine Mariette, Piotr Łaski, Radosław Kamiński, Katarzyna N. Jarzemska, Rachel Wallick, Renske van der Veen, Henrike Müller-Werkmeister, Gábor Molnár, Dao Xiang, Christopher Milne, Maciej Lorenc, Yifeng Jiang **R-6**
Capturing ultrafast dynamics in a nanocrystalline spin crossover thin film using femtosecond electron diffraction and X-ray diffraction
European XFEL, Schenefeld; Université de Toulouse; Shanghai Jiao Tong University; Uncharted Software, Toronto; Institute of Physics, Johannes Gutenberg University Mainz; Center for Data and Computing in Natural Sciences (CDCS), Hamburg; Deutsches Elektronen-Synchrotron DESY, Hamburg; European Synchrotron Radiation Facility, Grenoble; Department of Chemistry, University of Warsaw; Department of Chemistry, University of Illinois Urbana-Champaign; Helmholtz Zentrum Berlin für Materialien und Energie GmbH, Berlin; Institute of Chemistry, University of Potsdam; Institut de Physique de Rennes, Univ. Rennes; The University of Tokyo; Karlsruhe Institute of Technology, Institute of Microstructure Technology, Eggenstein-Leopoldshafen
- 12:15 – 12:45** **Minxue Tang**, Rachel Husband, Zuzana Konopkova, Cornelius Strohm **R-7**
Probing high-pressure phase transitions at intermediate strain rates using a dynamic diamond anvil cell at European XFEL
European XFEL; Deutsches Elektronen-Synchrotron DESY, Hamburg
- 12:45 – 13:00** **Ryszard Sobierajski**, Wojciech Gawęda, Adam Glinka, Katarzyna Jarzemska, Radosław Kamiński, Maciej Kozak, Jacek Kubicki, Dagmara Milewska **R-8**
XFEL – program wsparcia polskich naukowców
Instytut Fizyki PAN, Warszawa; Wydział Fizyki, Uniwersytet im. Adama Mickiewicza w Poznaniu; Wydział Chemii, Uniwersytet Warszawski; Narodowe Centrum Badań Jądrowych, Otwock-Świerk
- 13:00 – 13:15** **Radosław Kamiński** **R-9**
Current possibilities and further perspectives for crystallographers at EuXFEL
Wydział Chemii, Uniwersytet Warszawski
- 13:15 – 15:00** **PRZERWA / BREAK**

SESJA PLENARNA 3 / PLENARY SESSION 3

- 15:00 – 15:20 **Felix Hennersdorf** R-10
RIGAKU Advances in X-ray and Electron Crystallography
Rigaku Europe SE, Neu-Isenburg
- 15:20 – 15:30 **Kamil Urbański**, Barbara Puhr, Andrew Jones, Anderson Paiva R-11
Automated and Evacuated X-ray Optics for Improved Qualitative and Quantitative Phase Analysis
Anfon Paar Poland sp. z o.o., Warszawa; Anton Paar GmbH, Graz
- 15:30 – 15:50 **Vernon Smith** R-12
Crystallography using higher energy: advances in solid state, high-pressure analysis
Bruker AXS GmbH, Karlsruhe
- 15:50 – 16:10 **Sebastian Machowski** R-13
Analiza in situ ogniw akumulatorowych i charakterystyka materiałów akumulatorowych
Testchem, Radlin
- 16:10 – 16:30 Piotr Jakiela, Lei Ding, **Marcin Sadłowski** R-14
Dyfraktometr Empyrean 3 firmy Panalytical – przegląd możliwości pomiarowych z uwzględnieniem automatycznej optyki MultiCore
Malvern Panalytical B.V. Sp. z o. o., Warszawa; Malvern Panalytical B.V., Almelo
- 16:30 – 16:50 **Szymon Stolarek**, B. Lantz, A. Cheminal, F. Bossan, K. Joensen, S. Skou, A. Tutueanu, P. Hoghoj R-15
Xeuss - The Next Generation Beamline for Laboratory (GI-)SAXS/WAXS/USAXS
Xenocs SAS, Grenoble, Xenocs Inc, Holyoke; Xenocs Nordic, Kgs Lyngby
- 16:50 – 17:10 **Andrzej Wojtas** R-16
Presentation of PROTO manufacturing X-ray diffractometers
PROTO Manufacturing Europe
- 17:10 – 18:40 **SESJA PLAKATOWA A / POSTER SESSION A**
- 17:10 **Przekąski serwowane dzięki wsparciu Rigaku Europe SE**
Snacks served with the support of Rigaku Europe SE

Piątek, 28 czerwca 2024 r. / Friday, June 28, 2024

9:00 – 10:30 **SESJA PLAKATOWA B / POSTER SESSION B**

10:30 – 10:45 **PRZERWA / BREAK**

SESJA PLENARNA 4 / PLENARY SESSION 4

- 10:45 – 11:00 **Agnieszka J. Pietrzyk-Brzezińska**, Jakub Filipek, Katarzyna Chałaśkiewicz, Aleksandra Kośmider, Maciej Nielipiński, Agnieszka Michalak, Maria Bednarkiewicz, Mieszko Gośłowski-Żeligowski, Filip Prucnal, Bartosz Sekuła **R-17**
Diversity of the C-terminal domains in the TetR family of regulators
Institute of Molecular and Industrial Biotechnology, Lodz University of Technology;
Faculty of Biotechnology and Food Sciences, Lodz University of Technology
- 11:00 – 11:10 **Martyna Mateja-Pluta**, Agnieszka Kiliszek **R-18**
Stabilization of RNA structures using small molecules in crystallographic research
Institute of Bioorganic Chemistry, Polish Academy of Sciences, Poznań
- 11:10 – 11:25 **Wojciech Stawski**, Harry L. Anderson **R-19**
Self-assembly and flexibility of porphyrin nanorings in the solid state
Chemistry Research Laboratory, University of Oxford
- 11:25 – 11:40 **Mykhaylo Potopnyk**, Magdalena Ceborska, Roman Luboradzki, Stepan Kutsiy, Dmytro Volyniuk, Juozas V. Grazulevicius **R-20**
(Benzo)thiazole-based solid-state emissive N,O-chelated boron difluoride complexes
Institute of Organic Chemistry, Polish Academy of Sciences, Warsaw; Institute of Organic Chemistry, National Academy of Sciences of Ukraine, Kyiv; Faculty of Mathematics and Natural Sciences, Cardinal Stefan Wyszyński University in Warsaw; Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw; Department of Electronic Devices, Lviv Polytechnic National University; Department of Polymer Chemistry and Technology, Kaunas University of Technology
- 11:40 – 11:55 **Svitlana V. Shishkina**, Anna Shaposhnik, Mariia Shyshkina, Victoriya Dyakonenko **R-21**
Concomitant polymorphs as very suitable objects for studying of the principles of crystal formation
SSI Institute for Single Crystals NAS of Ukraine, Kharkiv;
- 11:55 – 12:05 **Mateusz Gołdyn**, Vânia André, M. Teresa Duarte, Margarida Susana, Clara S. B. Gomes **R-22**
Application of mechanochemistry in the preparation of novel praziquantel cocrystals: synthetic approach and structural analysis
Faculty of Chemistry, Adam Mickiewicz University of Poznań; Center for Advanced Technology, Adam Mickiewicz University in Poznań; Centro de Química Estrutural, Universidade de Lisboa; Associação do Instituto Superior Técnico para a Investigação e Desenvolvimento (IST-ID), Lisboa; LAQV-REQUIMTE, Department of Chemistry, NOVA University of Lisbon

- 12:05 – 12:20 Maciej Zieliński, Zbigniew Kaszukur, Wojciech Juszczyk R-23
The evolution of nanocrystalline catalyst surface structure under reaction conditions – an in-situ diffraction study
 Centrum Doskonałości NOMATEN, Narodowe Centrum Badań Jądrowych, Otwock-Świerk; Instytut Chemii Fizycznej PAN w Warszawie
- 12:20 – 12:35 Roman Gajda, Tomasz Poręba, Jan Parafiniuk, Mohamed Mezouar, Krzysztof Woźniak R-24
Hemimorfit – przemiana fazowa do struktury modulowanej pod wysokim ciśnieniem
 Department of Chemistry, University of Warsaw; European Synchrotron Radiation Facility (ESRF), Grenoble; Department of Geology, University of Warsaw
- 12:35 – 12:50 Piotr Rejnhardt, Roman Gajda, Jan Parafiniuk, Tomasz Poręba, Mohamed Mezouar, Przemysław Dera, Krzysztof Woźniak R-25
Tracing the mechanism of hydrogen-bond symmetrization in natrochalcite under high pressure by experimental charge density redistributions
 Department of Chemistry, University of Warsaw; Faculty of Geology, University of Warsaw; European Synchrotron Radiation Facility (ESRF), Grenoble; Hawai'i Institute of Geophysics and Planetology, Université d'hawaii à mānoa, Honolulu
- 12:50 – 13:00 Joanna Drwęska, Filip Formalik, Kornel Roztocki, Randall Q. Snurr, Leonard J. Barbour, Agnieszka Janiak R-26
CO₂ binding sites and temperature-induced structural transformations in CALF-20 metal-organic framework
 Faculty of Chemistry, Adam Mickiewicz University, Poznań
- 13:00 – 14:30 **PRZERWA / BREAK**
- SESJA PLENARNA 5 / PLENARY SESSION 5**
- 14:30 – 14:45 Anil Kumar, Paulina Maria Dominiak R-27
Determining the structure of organic molecules using high-resolution electron diffraction data from microcrystals: Insight from charge density analysis
 Faculty of Chemistry, University of Warsaw
- 14:45 – 14:55 Adrian Sulich, Jarosław Z. Domagała, Alexey Shekhovtsov, M.B. Kosmyna, Marek Berkowski, Wojciech Paszkowicz R-28
Extended defects in selected Ca₉RE(VO₄)₇, REVO₄ and Ca₃RE₂(BO₃)₄ single-crystals (RE = rare earth metal cation)
 Institute of Physics, Polish Academy of Sciences, Warsaw; Institute for Single Crystals, NASU, Kharkov
- 14:55 – 15:05 Anna Kaleta, A. Pedeches, H. Rotella, M-P. Chauvat, M. Morales, S.L. Delage, N. Delpuech, N. Michel, S. Kret, P. Dłuzewski, F. Semond, P. Ruterana R-29
Crystallographic TEM studies on NbN phases for metal-based transistors
 CIMAP, Caen; Université Côte d'Azur, SophiaAntipolis; III-V Lab, Palaiseau; Institute of Physics, Polish Academy of Sciences, Warsaw

- 15:05 – 15:15** **Maciej Zieliński**, Agata Zaborowska, Ryszard Diduszko, Fabio Di Fonzo, R-30
Lukasz Kurpaska
Temperature-induced phenomena in the Al₂O₃ anticorrosion coating of steel for lead-cooled nuclear reactors
NOMATEN Centre for Excellence, National Centre for Nuclear Research, Otwock-Świerk;
Istituto Italiano di Tecnologia, Milano; X-nano S.r.l, Milano
- 15:15 – 15:25** **Armand Budzianowski**, Karolina Pioruńska-Sędłak, R-31
Magdalena Popławska, Jan K. Maurin, Agata Błażewicz
Półilościowa analiza proszkowej dyfrakcji rentgenowskiej
Narodowe Centrum Badań Jądrowych, Otwock-Świerk;
Narodowy Instytut Leków, Warszawa
- 15:25 – 15:30** **WRĘCZENIE DYPLOMÓW ZA NAJLEPSZE PREZENTACJE
PLAKATOWE – ZAKOŃCZENIE KONWERSATORIUM
GRANTING DIPLOMAS FOR THE BEST POSTER PRESENTATIONS –
CLOSING CEREMONY**
- 15:30 – 17:00** **WALNE ZEBRANIE SPRAWOZDAWCZE POLSKIEGO TOWARZYSTWA
KRYSTALOGRAFICZNEGO / GENERAL ASSEMBLY MEETING OF
THE POLISH CRYSTALLOGRAPHIC ASSOCIATION**

PROGRAM SESJI NAUKOWEJ SEKCJI MŁODYCH KRYSTALOGRAFÓW POLSKIEGO TOWARZYSTWA KRYSTALOGRAFICZNEGO

PROGRAMME OF THE SCIENTIFIC SESSION OF THE YOUNG CRYSTALLOGRAPHERS SECTION OF THE POLISH CRYSTALLOGRAPHIC ASSOCIATION

Środa, 26 czerwca 2024 r. / Wednesday, June 26, 2024

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| 15:00 – 15:10 | <u>Alicja Pichlak</u> , Lucjan Jerzykiewicz, Tomasz Han
Oznaczenie zanieczyszczeń polimorficznych substancji czynnych z użyciem proszkowej dyfraktometrii rentgenowskiej
Wydział Chemii, Uniwersytet Wrocławski; Centrum Badawczo-Rozwojowe NOVASOME, Wrocław | M-1 |
| 15:10 – 15:20 | <u>Oskar Kaszubowski</u> , Katarzyna Ślepokura
Intermolecular interactions and supramolecular tendencies in crystals of adenosine monophosphate isomers
Faculty of Chemistry, University of Wrocław | M-2 |
| 15:20 – 15:30 | <u>Kateryna Kravets</u> , Laura Contini, Fabrizia Grepioni, Oksana Danylyuk
Host-guest assemblies of <i>p</i>-sulfonatocalix[n]arenes with benzamidines: solution versus slurry crystallization
Institute of Physical Chemistry Polish Academy of Sciences, Warsaw; Department of Chemistry "Giacomo Ciamician", University of Bologna | M-3 |
| 15:30 – 15:40 | <u>Monika Świniuch</u> , Błażej Dziuk, Renata Siedlecka
Analiza strukturalna kokryształów na bazie 1,4-bis(4-pirydylo)-1,3-butadienu pod kątem fotocykloaddycji [2+2]
Wydział Chemiczny, Politechnika Wrocławska | M-4 |
| 15:40 – 15:50 | <u>Aleksandra Zwolenik</u> , Anna Makal
Understanding the huge negative thermal expansion of 1,3-diacetylpyrene
Faculty of Chemistry, University of Warsaw | M-5 |
| 15:50 – 16:00 | <u>Anil Kumar</u> , Paulina Maria Dominiak
TAAM refinement on high-resolution experimental and simulated 3D ED/ MicroED data for organic molecules
Faculty of Chemistry, University of Warsaw | M-6 |
| 16:00 – 16:10 | <u>Paulina Maria Rybicka</u> , Marta Kulik, Michał Leszek Chodkiewicz, Paulina Maria Dominiak
The choice of local coordinate system and symmetry constraints – how they affect the local symmetry of atomic electron density?
Faculty of Chemistry, University of Warsaw | M-7 |

- 16:10 – 16:20 **Wojciech Stawski**, Harry L. Anderson M-8
Facts, myths and sandwiches: anions of [18]annulene
 Chemistry Research Laboratory, University of Oxford
- 16:20 – 16:30 **Vladyslav Maliuzhenko**, Marek Weselski, Janusz Gregoliński, M-9
 Robert Bronisz
Przemiana spinowa w rodzinie polimerów koordynacyjnych opartych o Fe(II) i *trans*-1,2-di(tetrazol-1-ylo)cyklopentan
 Wydział Chemii, Uniwersytet Wrocławski
- 16:30 – 16:40 **Karolina Matuszak**, Rafał Petrus, Vasyl Kinzhybalo M-10
Badania strukturalne aryloksylowych związków cynku w kontekście ich zastosowania w syntezie estrów alkilowych hydroksykwasów tłuszczowych
 Wydział Chemiczny, Politechnika Wroclawska; Instytut Niskich Temperatur i Badań Strukturalnych, Polska Akademia Nauk, Wrocław
- 16:40 – 16:50 **Kinga Potempa**, Damian Paliwoda, Katarzyna N. Jarzemska, Adam Krówczyński, Patryk Borowski, Michael Hanfland, Radosław Kamiński M-11
Unconventional binding mode of nitrite ligand opening up the possibility of pressure-driven linkage isomerism in piezochromic single crystals of nickel(ii) complex
 Department of Chemistry, University of Warsaw; European Spallation Source, Lund; European Synchrotron Radiation Facility, Grenoble
- 16:50 – 17:00 **Adrian Kowaliński**, Rafał Petrus M-12
Badania strukturalne dziewięciordzeniowych hydrokso klastrów metali ziem rzadkich
 Wydział Chemiczny, Politechnika Wroclawska
- 17:00 – 17:10 **Thi Thu Ha Nguyen**, Mane Sahakyan, Vinh Hung Tran M-13
Electronic structure and optical properties of Ba₂TiMnO₆: a DFT study
 University of the National Education Commission, Kraków; Institute of Low Temperature and Structure Research, Polish Academy of Sciences, Wrocław
- 17:10 – 17:20 **Adrian Sulich**, Jaroslaw Z. Domagala, Alexey Shekhovtsov, M-14
 M.B. Kosmyna, Marek Berkowski, Wojciech Paszkowicz
Extended defects in selected Ca₉RE(VO₄)₇, REVO₄ and Ca₃RE₂(BO₃)₄ single-crystals (RE = rare earth metal cation)
 Institute of Physics, Polish Academy of Sciences, Warsaw; Institute for Single Crystals, NASU, Kharkov