

PROGRAM KONWERSATORIUM

PROGRAM OF THE MEETING

Czwartek, 24 czerwca 2021 r. / Thursday, June 24, 2021

- 9:00 – 9:20 **Otwarcie Konwersatorium i uroczyste wręczenie nagród laureatom IV Ogólnopolskiej Olimpiady Krystalograficznej / Opening of the conference and the ceremonial awarding of prizes to the winners of the 4th Polish Crystallographic Olympiad**
- SESJA PLENARNA / PLENARY SESSION**
- 9:20 – 9:50 Angela B. Grommet, Oksana Yanshyna, Hema Kuntrapakam, Oleg V. Chashchikhin, **Michał J. Białek**, Rafał Klajna O-1
Faculty of Chemistry, Weizmann Institute of Science, Rehovot, Israel; Department of Chemistry, University of Wrocław
Host-guest interactions under molecular confinement within a flexible coordination cage – solid state vs. solution
- 9:50 – 10:10 **Piotr A. Guńka**, Janusz Zachara O-2
Wydział Chemiczny Politechniki Warszawskiej
Novel bond-valence-based coordination number definitions and their application to high-pressure crystal structures
- 10:10 – 10:30 **Jakub Drapała**, Radosław Kamiński, Krzysztof Durka, Katarzyna N. Jarzemska O-3
Warsaw University of Technology, Faculty of Chemistry: University of Warsaw, Faculty of Chemistry
Structural trends in bisphosphine complexes of coinage metals at first oxidation state
- 10:30 – 10:50 **Marta Otręba**, Katarzyna Ślepokura O-4
University of Wrocław, Faculty of Chemistry
Crystallochemical analysis of adenosine hypodiphosphate ester and related organic hypodiphosphates
- 10:50 – 11:00 **Kunal Kumar Jha**, Florian Kleemiss, Michał Leszek Chodkiewicz, Paulina M. Dominiak O-5
Electron Density Modelling Group, Department of Chemistry, University of Warsaw; Universität Regensburg, Fakultät für Chemie und Pharmazie, Regensburg, Germany
Aspherical atom refinements on X-ray and electron diffraction data of diverse structures including disorder and COF systems: a time-accuracy trade off
- 11:00 – 11:30 **PRZERWA / BREAK**

- 11:30 – 12:00 **Felix Hennersdorf, Marcus J. Winter** O-6
Rigaku Europe SE, Neu Isenburg, Germany
Rigaku advances in X-ray and electron crystallography
- 12:00 – 12:30 **Tadeusz Glenc** O-7
Testchem, Pszów
Prezentacja najnowszego dyfraktometru proszkowego firmy Rigaku
- 12:30 – 12:50 **Jarosław Serafińczuk** O-8
Department of Nanometrology, Wrocław University of Science and Technology;
Łukasiewicz Research Network – PORT Polish Center for Technology Development,
Wrocław
High resolution X-ray diffraction measurements carried out from the edge of the sample
- 13:00 – 14:00 **PRZERWA / BREAK**
- 14:00 – 14:20 Agnieszka Kiliszek, Leszek Błaszczuk, Magdalena Bejger, **Wojciech Rypniewski** O-9
Institute of Bioorganic Chemistry, Polish Academy of Sciences, Poznań
Broken symmetry between RNA enantiomers in a crystal lattice
- 14:20 – 14:40 **Joanna Loch**, Barbara Imiołczyk, Joanna Śliwiak, Anna Wantuch, O-10
Miroslaw Gilski, Mariusz Jaskólski
Jagiellonian University, Faculty of Chemistry, Kraków; Polish Academy of Sciences,
Institute of Bioorganic Chemistry, Poznań; A. Mickiewicz University, Faculty of Chemistry,
Poznań
Structural and functional studies of novel L-Asparaginase from *Rhizobium etli*
- 14:40 – 15:00 **Małgorzata K. Cabaj**, Paulina M. Dominiak O-11
Electron Density Modelling Group, Biological and Chemical Research Centre, Department
of Chemistry, University of Warsaw
Frequency and hydrogen bonding geometry of nucleobase homopairs in small molecule crystal structures
- 15:00 – 16:00 **Alexander Wlodawer**, Marek Grabowski, Joanna M. Macnar, Marcin O-12
Cymborowski, David R. Cooper, Ivan G. Shabalin, Miroslaw Gilski, Dariusz
Brzeziński, Marcin Kowiel, Zbigniew Dauter, Bernhard Rupp, Mariusz
Jaskólski, and Wladek Minor
Center for Structural Biology, National Cancer Institute, Frederick, MD, USA; Department
of Molecular Physiology and Biological Physics, University of Virginia, Charlottesville, VA,
USA; Faculty of Chemistry, University of Warsaw; Faculty of Chemistry, A. Mickiewicz
University, Poznań; Institute of Bioorganic Chemistry, Polish Academy of Sciences,
Poznań; Institute of Computing Science, Poznań University of Technology; k.-k
Hofkristallamt, San Diego, CA, USA; Institute of Genetic Epidemiology, Medical University
Innsbruck, Austria
One thousand structures of SARS-CoV-2 proteins, or how the Polish crystallographic mafia joined the fight against Covid-19
- 16:00 – 16:30 **PRZERWA / BREAK**
- 16:30 – 18:30 **SESJA PLAKATOWA A / POSTER SESSION A**

Piątek, 25 czerwca 2021 r. / Friday, June 25, 2021

SESJA PLENARNA / PLENARY SESSION

- 9:00 – 9:20 **Wiesław Świętnicki**, Ewa Brzozowska O-13
Instytut Immunologii i Terapii Doświadczalnej PAN im. L. Hirszfelda, Wrocław
Analiza *in silico* białek kanalikowych ogonka bakteriofaga sugeruje przypuszczalne miejsce wiązania cukru i mechanizm katalityczny
- 9:20 – 9:30 **Marta Kulik**, Michał L. Chodkiewicz, Paulina M. Dominiak O-14
Centrum Nauk Biologiczno-Chemicznych Uniwersytetu Warszawskiego, Wydział Chemii, Uniwersytet Warszawski
From electron density maps to electrostatic potential density maps of macromolecules with MATTS databank
- 9:30 – 9:40 **Anna Cociurovscaia**, Agnieszka Pietrzyk-Brzezińska O-15
Instytut Biotechnologii Molekularnej i Przemysłowej, Wydział Biotechnologii i Nauk o Żywności, Politechnika Łódzka
Identyfikacja potencjalnych efektorów bakteryjnego czynnika transkrypcyjnego RcdA
- 9:40 – 10:10 **Krzysztof Woźniak**, Marcin Stachowicz, Roman Gajda, Jan Parafiniuk O-16
Chemistry Department., University of Warsaw; Institute of Geochemistry, Mineralogy and Petrology, University of Warsaw
Experimental charge densities of minerals under pressure
- 10:10 – 10:20 **Daniel Tchoń**, Anna Makal O-17
Biological and Chemical Research Centre, Faculty of Chemistry, University of Warsaw
Completeness in high-pressure XRD experiments
- 10:20 – 10:30 **Svitlana V. Shishkina**, Yevhenii A. Vaksler, Abdenacer Idrissi O-18
SSI "Institute for Single Crystals" NAS of Ukraine, Kharkiv, Ukraine; V.N. Karazin Kharkiv National University, Kharkiv, Ukraine; Laboratoire de Spectroscopie pour les Interactions, la Réactivité et L'environnement, Université de Lille, Villeneuve d'Ascq, France
High-pressure influence on piracetam crystals: studying by quantum chemical methods
- 10:30 – 10:40 **Yevhenii A. Vaksler**, Abdenacer Idrissi, Svitlana V. Shishkina O-19
SSI "Institute for Single Crystals" NAS of Ukraine, Kharkiv, Ukraine; V.N. Karazin Kharkiv National University, Kharkiv, Ukraine; Laboratoire de Spectroscopie pour les Interactions, la Réactivité et L'environnement, Université de Lille, Villeneuve d'Ascq, France
Computational analysis of pressure-induced shear in R,S-ibuprofen
- 10:40 – 10:50 **Piotr Reinhardt**, Jan K. Zaręba, Ida Moszczyńska, Marek Daszkiewicz O-20
Institute of Low Temperature and Structure Research, Polish Academy of Sciences, Wrocław; Advanced Materials Engineering and Modelling Group, Faculty of Chemistry, Wrocław University of Science and Technology; Faculty of Chemistry, Adam Mickiewicz University, Poznań
Non-linear optical properties and negative area compressibility of (S)-2-amino-3-guanidinopropionic acid monochloride

- 10:50 – 11:00** **Michał Duda**, Marta Grzesiak-Nowak, Marcin Oszajca, Wiesław Łasocho **O-21**
Wydział Chemii Uniwersytetu Jagiellońskiego, Kraków; Instytut Katalizy i Fizykochemii Powierzchni im. Jerzego Habera PAN, Kraków
Synteza i badania strukturalne połączeń bromku kadmu z diaminami alifatycznymi z wykorzystaniem techniki rentgenowskiej dyfrakcji proszkowej
- 11:00 – 11:30** **PRZERWA / BREAK**
- 11:30 – 11:50** **Henryk Drozdowski**, Małgorzata Śliwińska-Bartkowiak, Stefan Jurga **O-22**
Faculty of Physics, Adam Mickiewicz University, Poznań
Application of crystallography in studies of soft materials
- 11:50 – 12:10** **Anna A. Hoser**, Marcin Sztylko, Anders Ø. Madsen **O-23**
Biological and Chemical Research Centre, Faculty of Chemistry, University of Warsaw; Department of Pharmacy, University of Copenhagen, Denmark
Theoretically derived thermodynamic properties can be improved by the refinement of low-frequency modes against X-ray diffraction data
- 12:10 – 12:35** **Iwona Lazar**, Andrzej Majchrowski, Krystian Roleder **O-24**
Institute of Physics, University of Silesia, Katowice; Institute of Applied Physics, Military University of Technology, Warsaw
Phase transitions in a $\text{PbZr}_{0.87}\text{Ti}_{0.13}\text{O}_3$ single crystal
- 12:35 – 12:50** **Irena Jankowska-Sumara**, Marek Paściak, Andrzej Majchrowski **O-25**
Institute of Physics, Pedagogical University of Cracow; Institute of Physics of the Czech Academy of Sciences, Prague, Czech Republic; Institute of Applied Physics, Military University of Technology, Warsaw
Modulated structures in $\text{Pb}(\text{Hf}_{1-x}\text{Sn}_x)\text{O}_3$ single crystals by X-ray diffraction
- 12:50 – 13:00** **Konrad Dyk**, Łukasz Baran, Wojciech Rżysko, Marek Stankevič, Daniel Kamiński **O-26**
Katedra Chemii Ogólnej, Koordynacyjnej i Krystalografii; Katedra Chemii Teoretycznej; Katedra Chemii Organicznej, Uniwersytet Marii Curie-Skłodowskiej w Lublinie
Wzajemne oddziaływanie między stabilnością kryształów a energią konformacji molekuly
- 13:00 – 14:00** **PRZERWA / BREAK**
- 14:00 – 16:00** **SESJA PLAKATOWA B / POSTER SESSION B**