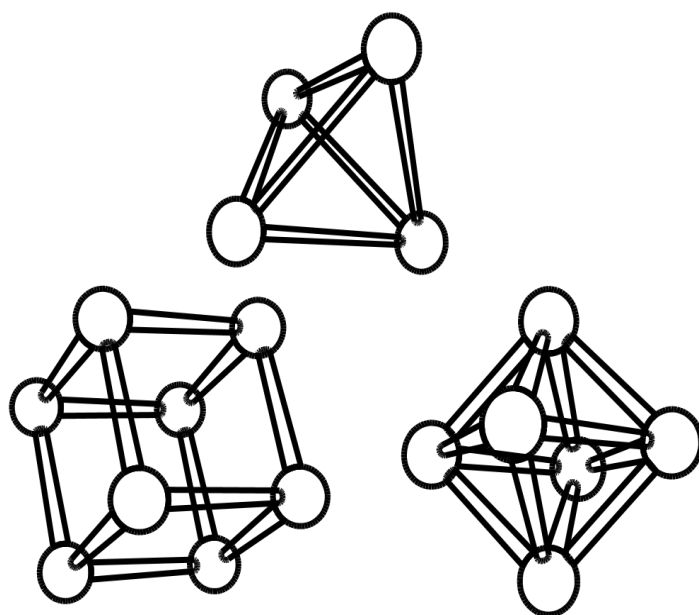


**CROATIAN CRYSTALLOGRAPHIC ASSOCIATION  
SLOVENIAN CRYSTALLOGRAPHIC SOCIETY**

# **THIRTIETH SLOVENIAN-CROATIAN CRYSTALLOGRAPHIC MEETING**



**12-16 June, 2024**

**Vitality hotel Punta**

**Veli Lošinj, Croatia**

# **PROGRAMME BOOK**

## **WEDNESDAY, June 12, 2024**

19<sup>00</sup> – 19<sup>30</sup> REGISTRATION OF PARTICIPANTS  
19<sup>30</sup> WELCOME RECEPTION

## **THURSDAY, June 13, 2024**

8<sup>00</sup> – 8<sup>45</sup> REGISTRATION OF PARTICIPANTS  
8<sup>45</sup> – 9<sup>00</sup> OPENING CEREMONY

**Chairpersons:** A. Meden, D. Matković-Čalogović

9<sup>00</sup> – 10<sup>00</sup> PLENARY LECTURE

**Ivan Halasz**

In situ powder X-ray diffraction and Raman spectroscopy for monitoring of ball-milling mechanochemistry

**Chairperson:** I. Đilović

10<sup>00</sup> – 10<sup>30</sup> COFFEE BREAK

SHORT PRESENTATIONS

**Chairpersons:** B. Kozlevčar, I. Đilović

10<sup>30</sup> – 10<sup>40</sup>

**Anton Meden**

X-Ray Powder Diffraction of High-Entropy alloys

10<sup>40</sup> – 10<sup>55</sup>

**Željko Skoko**, J. Popović, S. Popović

XRD "microscopy": a case of in-situ formation of the Al-Zn solid solution

10<sup>55</sup> – 11<sup>05</sup>

**Eugen Libowitzky**

Structure distortion of diamond-polished cuprite surface layers and its impact on Raman spectra

11<sup>05</sup> – 11<sup>15</sup>

**Ines Kulašić**, N. Petek, J. Svete, U. Grošelj, B. Štefane

Structural determination of novel pyrazolone and diazepine derivatives

11<sup>15</sup> – 11<sup>35</sup>

T. Strürzer, C. Lenczyk, J. Graf, **Martin Adam**

Bridging the gap between Electron and X-ray Diffraction

11<sup>45</sup> – 12<sup>00</sup>

BREAK

#### SHORT PRESENTATIONS

**Chairpersons:** N. Bedeković, P. Stanić

12<sup>00</sup> – 12<sup>10</sup>

**Nina Podjed**, Z. Uranjek, B. Modec

Zinc(II)-based coordination chemistry of furosemide: from complexes to coordination polymer

12<sup>10</sup> – 12<sup>25</sup>

**Matic A. Pipp**, N. Podjed, B. Modec

Zinc(ii) coordination polymer containing quinaldinate and 2-hydroxypyridine ligands

12<sup>25</sup> – 12<sup>35</sup>

**Mateja Pisačić**, B. Tokić, M. Đaković

Crystals under the spotlight – discovering the possibilities of crystals' dynamic behaviour

12<sup>35</sup> – 12<sup>45</sup>

**Uroš Rapuš**, J. Kljun, I. Turel

Suprising structure of a rhenium(I) complex

12<sup>45</sup> – 12<sup>55</sup>

**Marta Počkaj**, B. Košmrlj

Cobalt(III) complex with in situ formed ligand derived from 2-pyridinemethanol

12<sup>55</sup> – 13<sup>10</sup>

S. Marijan, T. Klaser, P. Mošner, L. Koudelka, Ž. Skoko, J. Pisk, **Luka Pavić**

Investigating the glass-forming region in sodium phosphate-niobate-based glass systems

13<sup>15</sup> – 15<sup>00</sup>

LUNCH BREAK

15<sup>00</sup> – 16<sup>00</sup>

PLENARY LECTURE

**Laura Cendron**

A structural view of SOS response in bacteria: how it works and how to block it

**Chairperson:** I. Kekez

16<sup>00</sup> – 16<sup>30</sup>

COFFEE BREAK

#### SHORT PRESENTATIONS

**Chairpersons:** I. Kekez, M. Počkaj

- 16<sup>30</sup> – 16<sup>45</sup> **Benoit Colasson**  
Supramolecular design for biomimetic model complexes: Crystallographic considerations from a non-crystallographer
- 16<sup>45</sup> – 16<sup>55</sup> **Jerneja Kladnik**, L. Rejc, D. Knez, G. Molina-Aguirre, A. Espargaró, A. Meden, L. Blinc, M. Lozinšek, R. D. Jansen-van Vuuren, M. Rogan, B. A. Martek, J. Mlakar, A. Dremelj, A. Petrič, S. Gobec, R. Sabaté, M. Bresjanac, B. Pinter, J. Košmrlj  
Fluorescent molecular probes for Alzheimer's diagnosis: Synthesis, crystal structures and biological evaluation
- 16<sup>55</sup> – 17<sup>10</sup> **Aleksandar Višnjevac**, I. Piantanida, O. Reinaud, B. Colasson  
Co(II) coordination by capped calix[6]arenes
- 17<sup>10</sup> – 17<sup>25</sup> **Žan Zakošek**, E. Goresnik  
Exploration of the ternary system CuBr – HBr – DABCO
- 17<sup>25</sup> – 17<sup>50</sup> BREAK
- 17<sup>50</sup> – 18<sup>00</sup> **Ana Siljanovska**, M. Virant, K. Molčanov, M. Lozinšek, J. Cerkovnik  
Hydrogen-bonded cocrystals of triphenylarsine oxide
- 18<sup>00</sup> – 18<sup>15</sup> **Nikola Bedeković**, A. Magnabosco, V. Stilinović, D. Cinić  
Pyridine nitrogen as a bifurcated halogen bond acceptor in cocrystals of 1,2-diodotetrafluorobenzene and pyridine derivatives: CSD survey, structural and computational study
- 18<sup>15</sup> – 18<sup>35</sup> **Vladimir Stilinović**, N. Baus Topić, E. Topić, L. Fotović  
Morphotropism in a series of halogen bonded cocrystals derived from an isomorphous series of *N*-(4-halobenzyl)-3-halopyridinium halogenides
- 18<sup>35</sup> – 18<sup>45</sup> **Matic Lozinšek**  
Crystal structure of spicy capsaicin
- 19<sup>00</sup> – 20<sup>30</sup> **Matthew Lightfoot, Lily Hunnisett**  
CSD WORKSHOP: unlocking new insights thanks to over a million structures

## **FRIDAY, June 14, 2024**

- 9<sup>00</sup> – 10<sup>00</sup> PLENARY LECTURE  
**Damjan Pelc**  
Diffuse scattering and nanoscale correlations in quantum materials  
**Chairperson:** M. Lozinšek

10<sup>00</sup> – 10<sup>30</sup>

COFFEE BREAK

SHORT PRESENTATIONS

**Chairpersons:** M. Pisačić, M. Lozinšek

10<sup>30</sup> – 10<sup>50</sup>

**Jakub Wojciechowski (Rigaku)**

Improving workflows in CrysAlisPro with intelligent devices and automations

10<sup>50</sup> – 11<sup>00</sup>

**Bogdan Kotur**, V. Babizhetskyy, C. Zheng, V. Smetana

New ternary gallide Zr<sub>7</sub>Pd<sub>7-x</sub>Ga<sub>3+x</sub> (0 ≤ x ≤ 1.8)

11<sup>00</sup> – 11<sup>10</sup>

**Lia Šibav**, M. Lozinšek, Z. Jagličić, A. Zorko, M. Dragomir

Crystal growth, structural and magnetic characterisation of ErTa<sub>7</sub>O<sub>19</sub> and Er<sub>3</sub>Ta<sub>17</sub>O<sub>47</sub>

11<sup>10</sup> – 11<sup>20</sup>

**Petra Stanić**, K. Molčanov

Quantum crystallographic study of pancake-bonded TCNQ radical anions

11<sup>20</sup> – 11<sup>40</sup>

**Krešimir Molčanov**, P. Stanić, L. Molčanov, M. Jurić, F. Meurer, M.

Bodensteiner, C. Hennig, M. Virant, M. Lozinšek

Two-electron multicentre bonding (pancake bonding): from discrete dimers to extended 2D arrays

11<sup>50</sup> – 12<sup>00</sup>

BREAK

**Chairpersons:** L. Molčanov, J. Jakoš

12<sup>00</sup> – 12<sup>20</sup>

**M. Arhangelskis**, Y. Xu, M. L. Chodkiewicz, M. Woińska, D. Trzybiński, I. Brekalo, F. Topić, K. Woźniak

Hirshfeld atom refinement for metal-organic frameworks: accurate assignment of hydrogen atom positions and detailed analysis of guest disorder

12<sup>20</sup> – 12<sup>40</sup>

**Viktoriiia Drushliak**, M. Szafranski

High-Pressure and Temperature Studies Open New Insights into Two-Dimensional Perovskite CsC[(NH<sub>2</sub>)<sub>3</sub>]PbI<sub>4</sub>

12<sup>40</sup> – 12<sup>55</sup>

**Yizhi Xu**, J. Dorrell, J. P. Darby, J. M. Marrett, H. M. Titi, A. J. Morris, T. Friščić, M. Arhangelskis

High throughput ab initio crystal structure prediction of metal-organic frameworks with machine learning

12<sup>55</sup> – 13<sup>05</sup>

**Lily M. Hunnisett**, J. Nyman, N. Francia, G. Sadiq, I. Sugden, J. Cole  
A Seventh Blind Test of Crystal Structure Prediction Methods

13<sup>05</sup> – 13<sup>15</sup>

**Jure Jakoš**, A. Juvan, M. Pesek, M. Marolt, J. Košmrlj, M. Gazvoda

Structure elucidation of organic molecules from experimental spectroscopic data using Schmarnica

13<sup>15</sup> – 15<sup>45</sup>

LUNCH BREAK

15<sup>45</sup> – 19<sup>30</sup>

**Conference trip**

(visit the Museum of Apoxyomenos and Lošinj's Fragrant Garden)

## **SATURDAY, June 15, 2024**

9<sup>00</sup> – 10<sup>00</sup>

PLENARY LECTURE

**Catharine Esterhuysen**

The role of intermolecular interactions in chemical processes

**Chairperson:** M. Đaković

10<sup>00</sup> – 10<sup>30</sup>

COFFEE BREAK

SHORT PRESENTATIONS

**Chairpersons:** M. Đaković, Ž. Skoko

10<sup>30</sup> – 10<sup>40</sup>

**Mario Cetina**, A. Meščić, S. Raić-Malić

Supramolecular architectures of two N-acyclic uracil derivatives

10<sup>40</sup> – 10<sup>55</sup>

**Christopher J. Kingsbury**, I. J. Sugden

Aromatics Analyser 2 and a unified approach to aromatic interactions

10<sup>55</sup> – 11<sup>05</sup>

**Andreas Ertl**

A FIRST ATTEMPT TO USE CORRELATIONS IN TOURMALINE AS A THERMOMETER

11<sup>05</sup> – 11<sup>20</sup>

**Dominik Talla**, Ž. Zakošek, G. Giester

The single-diffusion gel growth technique: a way of preparing novel metal-organic complexes

11<sup>20</sup> – 11<sup>30</sup>

**Žan Zakošek**, D. Talla, G. Giester, M. Počkaj

Coordination compounds with indole-2- and indole-3-carboxylates

11<sup>30</sup> – 10<sup>45</sup>

**Mirjana M. Radanović**, M. S. Kostić, M. V. Rodić, N. D. Radnović, Lj. S. Vojinović-Ješić, F. Perdih

Synthesis and structure of Cu(I) complex with Schiff base of aminoguanidine and 2-(diphenylphosphino)benzaldehyde

11<sup>45</sup> – 12<sup>00</sup>

BREAK

**Chairpersons:** K. Molčanov, G. Giester

- 12<sup>00</sup> – 12<sup>10</sup> **Andrii Hultiaiev**, E. Goreshnik  
The new Cu(I)-Cl-polyamine compounds
- 12<sup>10</sup> – 12<sup>20</sup> **Erik Uran**, K. Radan, M. Virant, M. Dragomir, M. Lozinšek  
Reactivity of cyanogen towards [XeF]<sup>+</sup> cation
- 12<sup>20</sup> – 12<sup>30</sup> **Miha Virant**, V. Milašinović, K. Radan, M. Lozinšek  
Coordination of carbamoyl fluoride to fluoridoxenon(1+) cation
- 12<sup>30</sup> – 12<sup>40</sup> **Viktorija R. Kukharuk**, V. N. Kokozay, E. A. Goreshnik, S. R. Petrusenko  
(*E*)-*N'*-((5-(hydroxymethyl)furan-2-yl)methylene) benzohydrazide and its copper(ii) complex: synthesis and crystal structure
- 12<sup>40</sup> – 12<sup>55</sup> **Evgeny Goreshnik**, S. Petrusenko  
Diversity of mixed cupro(i)-cyano-thiocyanato anionic polymers
- 12<sup>55</sup> – 13<sup>10</sup> **Bojan Kozlevčar**, A. Pevec  
Coordination compounds with 5-sulfosalicylates
- 13<sup>15</sup> – 15<sup>00</sup> LUNCH BREAK
- 15<sup>00</sup> – 16<sup>00</sup> PLENARY LECTURE  
**Mirela Dragomir**  
Synthesis and structure-property relationships of selected quantum materials  
**Chairperson:** V. Stilinović
- 16<sup>00</sup> – 16<sup>30</sup> COFFEE BREAK
- 16<sup>30</sup> – 16<sup>40</sup> **Klemen Motaln**, M. Lozinšek  
On the synthesis and structure of salts containing the peculiar [MF<sub>3</sub>(XeF<sub>2</sub>)<sub>3</sub>]<sup>+</sup> (M = Pd, Pt) cations
- 16<sup>40</sup> – 16<sup>50</sup> **Olha Sanko**, E. Uran, K. Radan, M. Lozinšek  
Synthesis and Structural Analysis of Novel Xell–N-bonded Compounds
- 16<sup>50</sup> – 17<sup>00</sup> **Monika Šoltić**, N. Baran, I. Marić, G. Štefanić, M. Marciuš, G. Dražić, R. Peter, T. Jurkin, M. Ivanda, M. Gotić  
Synthesis, characterization and gas sensing properties of platinum nanoparticles dispersed on iron oxide support
- 17<sup>00</sup> – 17<sup>15</sup> **Matjaž Kristl**, B. Dojer, T. M. Podnar, A. Golobič  
Crystal structures of novel copper coordination compounds with pyridinecarbonitriles

17 <sup>15</sup> – 17 <sup>25</sup>	BREAK
17 <sup>25</sup> – 17 <sup>35</sup>	<b>Mišel Hozjan</b> , F. Perdih Zinc complexes with derivatives of picolinic acid
17 <sup>35</sup> – 17 <sup>45</sup>	<b>Kristian Radan</b> , L. Clough, S. Parsons, M. Lozinšek Recent advances in coordination chemistry of metal complexes with XeF <sub>2</sub> as a ligand
17 <sup>45</sup> – 18 <sup>00</sup>	<b>Marijana Đaković</b> , M. Borovina, M. Pisačić, M. Zausnig, I. Kodrin Structure-property relationship in mechanoflexible crystalline coordination polymers
18 <sup>00</sup> – 18 <sup>30</sup>	CLOSING REMARKS <b>Chairpersons:</b> A. Meden, D. Matković-Čalogović
20 <sup>00</sup>	CONFERENCE DINNER

### **SUNDAY, June 16, 2024**

9 <sup>00</sup>	EVALUATION AND FAREWELL COFFEE
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