BOOK OF ABSTRACTS

25th International Conference on the Chemistry of the Organic Solid State (ICCOSS XXV)

"(Re)building bridges in the solid-state research community"

July 3 – 8, 2022, Hotel Inex Olgica, Ohrid, Macedonia

CONTENTS

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Monday, July 4	**Morning Session**
08:00	**Registration desk open,** Hotel lobby
07:30-08:40	**Breakfast**, Hotel restaurant
SESSION 1: CRYSTALS THAT MOVE AND DEFORM	
08:40	**Session overview**
09:00	**Marijana Đaković**, University of Zagreb, Croatia *A Maze of Crystal Adaptability*
09:40	**Hideko Koshima**, Waseda University, Japan *Light-Driven Crystal Actuation*
10:20-11:00	**Coffee Break**
11:00	**Luca Catalano**, Université Libre de Bruxelles, Belgium *Understanding Martensitic Organic Crystals: from Molecular Dynamics to Macroscopic Motion*
11:40	**Kana M. Sureshan**, IISER Thiruvananthapuram, India *Topochemical Reaction Led Mechanical Responses*
12:00	**Željko Skoko**, University of Zagreb, Croatia *Do Crystals Need to Shrink in Order to Jump?*
12:20-13:30	**Lunch, hotel restaurant / terrace**

Monday, July 4	**Afternoon Session**
SESSION 2: CRYSTALS IN COMPUTERS	
13:30	**Session overview**
13:50	**Carole Morrison**, University of Edinburgh, UK *Towards the Rational Design of Energetic Materials with Tailored Impact Sensitivities*
14:30	**Martijn Zwijnenburg**, University College London, UK *The Emergence of Electronic and Optical Properties in Organic Materials Arising from the Structural Organisation of Organic Building Blocks*
15:10-15:40	**Coffee Break**
15:40	**Snežana Zarić**, University of Belgrade, Serbia *Interactions of Aromatic Rings in Crystal Structures*
16:20	**Ljupčo Pejov**, Ss. Cyril and Methodius University, Macedonia *Structural Perturbations and Vibrational Spectra of Bent Molecular Crystals: Periodic DFT Coupled with Multivariate Statistics Approach*
16:40	**Marta Dudek**, Polish Academy of Sciences, Poland *Determination of Molecular Conformation in Organic Crystals using Combined Crystal Structure Prediction (CSP) – Solid State NMR Approach*
17:00 – 19:00	**Poster Session A (odd numbers)** Diamond Hall
19:00	**Dinner** (Hotel restaurant)
20:00	**Macedonian folk dance performance** (Hotel terrace)

Tuesday, July 5	**Morning Session**
08:00	**Registration,** Hotel lobby
07:30-08:40	**Breakfast,** Hotel resturant
SESSION 1: CRYSTALS THAT GROW	
08:40	**Session overview**
09:00	**Peter Vekilov**, University of Houston, USA *The Elementary Reactions for Incorporation into Crystals*
09:40	**Magalí Lingenfelder**, Max Planck-EPFL, Switzerland *Proteins that Grow on Surfaces: from Single Molecules to Medicine*
10:20-11:00	**Coffee Break**
11:00	**Assaf Gal**, Weizmann Institute of Science, Israel *Mechanisms of Biological Control over Crystal Morphogenesis*
11:40	**Marieh Al-Handawi**, New York University Abu Dhabi, UAE *Harvesting of Aerial Water by Hygroscopic Salt Excrections of the Desert Shrub Tamarix aphylla*
12:00	**Leah Javitt**, Weizmann Institute of Science, Israel *The Chemical Nature of Electrofreezing of Super Cooled Water*
12:20-13:30	**Group Photo – Hotel terrace** **Lunch – Hotel restaurant / terrace**

Tuesday, July 5	**Afternoon Session**
SESSION 2: CRYSTALS FOR DEVICES	
13:30	**Session overview**
13:50	**Rajadurai Chandrasekar**, University of Hyderabad, India *Mechanophotonics: A Roadmap to All-Organic Photonic Integrated Circuits from Nano/Micro Organic Solids*
14:30	**Delia Haynes**, Stellenbosch University, South Africa *Towards Functional Materials with Dithiadiazolyl Building Blocks*
15:10-15:40	**Coffee Break**
15:40	**Helena Shepherd**, University of Kent, UK *Solid-State Switching of Donor-Acceptor Stenhouse Adducts*
16:20	**Hagai Cohen**, Weizmann Institute of Science, Israel *Consequences of the Semi-Gap in Metal Free Perovskite Crystals*
16:40	**Amit Mondal**, IISER Kolkata, India *Metal-Like Ductility and Malleability in Organic Plastic Crystals*
17:00 – 19:00	**Poster Session B (even numbers),** Diamond Hall
17:30 – 18:30	**ICCOSS Advisory Board meeting, Golden Hall / online hybrid meeting**
19:30	**Boat cruise and light dinner on boat**

Wednesday, July 6	**Morning Session**
08:00	**Registration,** Hotel lobby
07:30-08:40	**Breakfast,** Hotel resturant
SESSION: CRYSTALS IN NATURE & MEDICINE	
08:40	**Session overview**
09:00	**Kevin Roberts**, University of Leeds, UK *Molecular, Solid-State and Surface Structures of the Conformational Polymorphic Forms of Ritonavir in Relation to their Physicochemical Properties*
09:40	**Jessica Bruhn,** NanoImaging Services, USA *Structure Determination via MicroED in the Pharmaceutical Industry: Lessons Learned from Solving 50+ Structures*
10:20-11:00	**Coffee Break**
11:00	**James De Yoreo**, University of Washington, USA *An in situ Look at Interfacial Controls on Crystallization in Biomolecular and Biomimetic Systems*
11:40	**Tomče Runčevski**, Southern Methodist University, USA *Titan in a Jar*
12:00	**Gérard Coquerel**, Université de Rouen Normandy, France *Transfer of Chirality: from a Single Supramolecular Chirality in Crystals to a Stereospecific Crystallization in a Conglomerate Forming System*
12:40	**Boat trip to the St. Naum Monastery**

14:00	**Lunch, Resturant at the St. Naum Monastery**
16:30	**Boat leaves the site to the hotel**
19:00	**Dinner at the hotel resturant**
18:00	**Advisory Board members reception (by invitation only)**

Thursday, July 7	**Morning Session**
08:00	**Registration,** Hotel lobby
07:30-08:40	**Breakfast,** Hotel resturant
SESSION 1: CRYSTALS UNDER LIGHT AND FORCE	
08:40	**Session overview**
09:00	**James Mack**, University of Cincinnati, USA *Mechanochemistry is Just Chemistry*
09:40	**Len MacGillivray**, University of Iowa, USA *Building Molecules in Crystals*
10:20-11:00	**Coffee Break**
11:00	**Calvin Sun**, University of Minnesota, USA *Crystallographic Origin of the Contrasting Deformation Behaviors of a Molecular Crystal During 3 Point Bending and Powder Compaction*
11:40	**Manas Kumar Panda**, Jadavpur University, India *Light-Fueled Macroscopic Motion by Organic Crystals*
12:00	**Manuel Fernandes**, University of Witwatersrand, South Africa *Activating the Thermosalient Effect in Crystals by Photochemical Reaction*
12:20-13:30	**Lunch – Hotel restaurant / terrace**

Thursday, July 7	**Afternoon Session**
SESSION 2: CRYSTAL SURFACES AND INTERFACES	
13:30	**Session overview**
13:50	**Franziska Emmerling**, Federal Institute for Materials Research and Testing (BAM), Germany *Mechanochemical Formation of Multicomponent Crystal Systems: Mechanism & Kinetics*
14:30	**Maria Chiara di Gregorio**, Weizmann Institute of Science, Israel *Metal-Organic Crystals: Shaping, Uniformity and Symmetry Breaking*
15:10-15:40	**Coffee Break**
15:40	**Igor Sokolov**, Tufts School of Engineering, USA *Detection of Different Phases of Polymer Material Using New Modes of Atomic Force Microscopy*
16:20	**Alexei Tivanski**, University of Iowa, USA *The effect of Nanosizing on Mechanical Properties of Organic Crystalline Solids*
16:40	**Sharmarke Mohamed**, Khalifa University of Science and Technology, UAE *Is Mechanochemistry Biased Towards Thermodynamic Products of Crystallization? Insights from Experimental and Computational Methods*
17:30	**Dinner in town, Buses leave from hotel to town**
21:30	**Return to hotel / Explore the Ohrid nightlife Buses leave from hotel to town**

Friday, July 8	**Morning Session**
08:00	**Registration,** Hotel lobby
07:30-08:40	**Breakfast,** Hotel resturant
SESSION 1: CRYSTALS WITH HOLES	
08:40	**Session overview**
09:00	**Miguel A. Garcia-Garibay**, UCLA, USA *Emergent Properties of Molecular Dipolar Arrays*
09:40	**Kim Jelfs**, Imperial College London, UK *Unravelling the Effects of Defects and Disorder in Porous Materials through Computation*
10:20-11:00	**Coffee Break**
11:00	**Ognjen Miljanić**, University of Houston, USA *Greenhouse Gas Capture in Porous Molecular Crystals*
11:40	**Consiglia Tedesco**, University of Salerno, Italy *Cyclic Peptoids: a Playground for Non-Covalent Interactions*
12:00	**Jason Benedict,** University of Buffalo, USA *Diarylethene-Based Crystalline Materials: Design and Function*
12:20-13:30	**Lunch – Hotel restaurant / terrace**

Friday, July 8	**Afternoon Session**
SESSION 2: CRYSTALS AND METHODS	
13:30	**Session overview**
13:50	**Kenneth Harris**, Cardiff University, UK *Structure Determination of Organic Materials from Powder X-ray Diffraction Data: Opportunities for Multi-technique Synergy*
14:30	**Ute Kolb**, Technische Universität Darmstadt, Germany *Automated Diffraction Tomography – Solving Crystal Structures of Beam and Vacuum Sensitive Organics*
15:10-15:40	**Coffee Break**
15:40	**Adam A. L. Michalchuk**, Federal Institute for Materials Research and Testing (BAM) *Time Resolved in situ Monitoring of Mechanochemical Transformations*
16:20	**Suzanna Ward**, CCDC, UK *Fun and Engaging Ways to Share the Wonders of Crystallography*
16:40	**Christian Göb**, Rigaku *Structure Determination of Small Molecule Compounds by an Electron Diffractometer for 3D ED/MicroED*
17:00	**Plenary Lecture 3: Masako Kato**, Kwansei Gakuin University, Japan *Photofunctional Soft Crystals Based on Platinum(II) Complexes*

18:00	**Pleanary Lecture 4: Len Barbour**, Stellenbosch University, South Africa *(Title TBA)*
19:00	**Closing remarks**
19:15	**Dinner** (Hotel restaurant)

Saturday, July 2	**Workshop**
WORKSHOP: Neutron and X-ray Methods for Structural Analysis of Organic Materials (pre-registration required) Golden Hall (hotel basement)	
07:30-09:00	**Breakfast,** Hotel restaurant
09:00	**Workshop overview, Tomče Runčevski**
09:15	**Mirijam Zobel,** RWTH Aachen University, Germany *Recent Advances in Laboratory PDF Experiments*
09:55	**Maxwell Terban**, Max Planck Institute for Solid State Research, Germany *Insights into Organic Materials Using the Pair Distribution Function*
10:35-11:00	**Coffee Break (workshop participants only)**
11:00	**Robert Dinnebier**, Max Planck Institute for Solid State Research, Germany *X-ray Powder Diffraction in Education*
11:40	**Sebastian Bette**, Max Planck Institute for Solid State Research, Germany *XRPD data Analysis of Stacking Faulted, Organic Materials*
12:20	**Thomas Blanton,** International Centre for Diffraction Data (ICDD) *Advanced Materials Characterization Using Powder Diffraction Techniques and the Powder Diffraction File*
13:00-14:00	**Lunch-Hotel restaurant / terrace**

P-7 The Correlation of the *p*K_a Equalization Principle to Charge-Assisted Hydrogen Bonds in Differentiation of the Molecular Salts from Cocrystals

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On the basis of the *p*K_a equalization principle, the strongest hydrogen bonds are associated with a very low Δ*p*K_a value, i.e. the difference between donor and acceptor acidic constants. [1] The Δ*p*K_a value associated with a general D—H···A interaction is calculated as Δ*p*K_a (D—H···A) = *p*KAH (D—H) ─ *p*K+BH(A—H+) is applied to correlate the wide range O···N distance distribution to chemical diversity, expressed in terms of acidity constant, displayed by the conformer molecules in Phloroglucinol (PHL) cocrystals and pyridoxime (vitamin B6) molecular salts. [2,3]. The presented crystal structure packing motifs between cocrystallized, both neutral *N*-heterocycles coformers and O-type of acidic drug model (PHL), as well between protonated and non-protonated N-heterocycle (pyridine type of drug model pyridoxine) and aromatic carboxylic acids confirm that the bond distances correlate to the nature of the hydrogen bond in range from week charge-assisted H-bonds in PHL/N-heterocycles cocrystals (Δ*p*K_a < 0), toward the so-called “salt–cocrystal continuum” in unprotonated pyridine derivative (Δ*p*K_a 0 – 1), till to formation strong charge-assisted H-bonds in molecular salts of the same protonated pyridine (Δ*p*K_a > 3). [4]

References:

[1] Gilli, P., Pretto, L., Bertolasi, V. & Gilli, G. (2009). Acc. Chem. Res. 42, 33–44
[2] Cvetkovski, A., Bertolasi, V. Ferretti, V. Acta Cryst. (2016). B72, 326–334.
[3] Cvetkovski, A., Ferretti, V. & Bertolasi, V. (2017). *Acta Cryst.* C73, 1064–1070.
[4] Aitipamula, S., *et al.*, *Crystal Growth & Design* (2012) *12* (5), 2147-2152