



Parma, September 6-9, 2021

Programme and Book of Abstracts





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SCHEDULE

Monday 6th September

8:30-9:00 Congress Opening

Alessia Bacchi, Scientific Committee
Chiara Massera, Organising Committee
Paolo Pio Mazzeo, Organising Committee

9.00-10:00 Plenary lecture [Chair: Alessia Bacchi (Università di Parma)]

Marijana Đaković, Zagreb University (Croatia)

Mechanically responsive molecular crystals

MS1: Crystallography of minerals and synthetic analogues

Chairs: Gianni Andreozzi (Università Roma La Sapienza), Marta Morana (Università di Pavia)

Invited talks:

10:30-11:00 KN1 Tiziana Boffa Ballaran, University of Bayreuth

A crystallographic view of the Earth's mantle

11:00-11:30 KN2 Ferdinando Bosi, Sapienza University of Rome

What do we mean by mineral species?

Oral presentations:

11:30-11:50 O1 Francesco Pagliaro - *High-pressure behavior and crystal chemistry of natural REE-bearing arsenates and phosphate*

11:50-12:10 O2 Giovanni Orazio Lepore - *Short-range order of tunnel cations in hollandite supergroup minerals*

12:10-12:30 O3 Maria Chiara Dalconi - *A new calcium aluminate phase containing formate from the cement industry*

MS2: Non-covalent interactions in crystals

Chairs: Consiglia Tedesco (Università di Salerno), Luca Catalano (Université Libre de Bruxelles)

Invited talks:

10:30-11:00 KN1 Antonio Frontera, University of Balearic Islands

Structure guiding role of σ -hole interactions in X-ray structures

11:00-11:30 KN2 Patrizia Rossi, Università di Firenze

Investigating NSAIDs salts: A solid-state point of view

Oral presentations:

11:30-11:50 O1 Fabio Montisci - *Cocrystallization of Essential Oils for Food Preservation and Agriculture*

11:50-12:10 O2 Emanuele Priola - *Solid-state peculiarities and polymorphism in imidazo[1,5- α]pyridine dyes*

12:10-12:30 O3 Marco Moroni - *Bipyrazolate MOF phase transition driven by adsorbent-adsorbate non covalent interactions: a multi-technique investigation*

12:30-14:30 Poster Session 1 (MS1-MS4)

MS3: Innovative functional materials: crystal growth and properties

Chairs: Antonio Vecchione (CNR-SPIN, Salerno), Paola Prete (CNR-IMM, Lecce)

Invited talks:

14:30-15:00 KN1 Enrico Giannini, University of Geneva

Magnetic van der Waals materials: structures and physical properties

15:00-15:30 KN2 Christian Kranert, IISB Fraunhofer

Facet Growth and Geometry of the Growth Ridge During Dynamic Czochralski Processes

Oral presentations:

15:30-15:50 O1 Paola De Padova - *The Importance of Being Silicene*

15:50-16:10 O2 Piero Mazzolini - *Ga₂O₃ polymorphs: tailoring the epitaxial growth conditions*

16:10-16:30 O3 Andrea Sala - *Photovoltaic varnishes: chalcogenide based thin film solar cells by ultra-low-cost ball milling*

MS4: Hot topics in macromolecular crystallography

Chairs: Giusy Tassone (Università di Siena), Massimo Degano (HSR, Milano)

Invited talks:

14:30-15:00 KN1 Andrea Mattevi, Università di Pavia

NADPH Oxidase: Structure, enzymology and drug design

15:00-15:30 KN2 KN2 Andrea Ilari, IBPM-CNR Roma

Trypanothione Reductase: one target, different approaches for the development of a broad-spectrum trypanocidal drug

Oral presentations:

15:30-15:50 O1 Vincenzo Mangini - *Structural investigations on the interplay between metal ions targeting proteins involved in copper homeostasis*

15:50-16:10 O2 Ludovica Lopresti - *Structural characterization of YAP-TEAD4 protein-protein interaction: an emerging target for cancer treatment*

16:10-16:30 O3 Silvia Fanti - *Structural insights into the Catalytic Site of Phosphoribulokinase from the green microalga Chlamydomonas Reinhardtii*

17:00-18:00 Plenary lecture [**Chairs:** Roberto Fornari (Università di Parma), Andrea Zappettini (IMEM-CNR)]

Juan Manuel Garcia Ruiz, University of Granada (Spain)

The Crystal and the Rose: The impact of crystals and crystallography on art and mind

Tuesday 7th September

9:00-10:00 Plenary lecture [**Chair:** Sabrina Nazzareni (Università di Perugia)]

Mohamed Mezouar, ESRF, Grenoble (France)

Revealing Phase Transitions and the Emergence of Structural Complexity at the ESRF Extremely Brilliant Source

MS5: Integration of diffraction techniques in structural biology

Chairs: Alessandro Grinzato (Università di Padova), Marina Mapelli (IEO – Milano)

Invited talks:

10:30-11:00 KN1 Federico Forneris, Università di Pavia

The molecular diversity of collagen lysine post-translational modification enzymes

11:00-11:30 KN2 Montse Soler Lopez, ESRF Grenoble

Integrative biology to unlock the secrets of protein complexes

Oral presentations:

11:30-11:50 O1 Marco Nardini - *Structural Basis of Inhibition of the Pioneer Transcription Factor NF-Y*

11:50-12:10 O2 Giorgio Giardina - *Cryptic functions and the need for imperfection*

12:10-12:30 O3 Martino Bolognesi - *Mapping ion permeation, gating, and drug binding in the HCN4 pacemaker channel*

MS6: Frontiers in Methods and Techniques for crystal structure characterization

Chairs: Benedetta Carrozzini (IC-CNR, Bari), Paolo Mazzeo (Università di Parma)

Invited talks:

10:30-11:00 KN1 Carlotta Giacobbe, ESRF, Grenoble

Extremely Brilliant Sources and opportunities. Are we really prepared?

11:00-11:30 KN2 Piero Macchi, Politecnico di Milano

The connubium between crystallography and quantum mechanics

Oral presentations:

11:30-11:50 O1 Nicola Corriero - *Machine Learning approach for symmetry prediction from X-ray powder diffraction patterns*

11:50-12:10 O2 Giulio Lampronti - *Reversible quantitative interconversion of three polymorphs by ball mill grinding: subtle control of relative polymorph stabilities*

12:10-12:30 O3 Stefano Racioppi - *A Topological Approach to the Electronegativity of Atoms in Molecules and Crystals*

12:30-14:30 Poster Session 2 (MS6-MS8)

MS7: Structure, function, application and dynamics of porous and nonporous crystals

Chairs: Donatella Armentano (Università della Calabria), Stefano Canossa (Antwerp University)

Invited talks:

14:30-15:00 KN1 Marco Taddei, Università di Pisa

Atomic-level description of the cooperative CO₂ adsorption behaviour in a perfluorinated metal-organic framework

15:00-15:30 KN2 Nuria Martín, University of Valencia

Porous crystalline materials for catalytic applications

Oral presentations:

15:30-15:50 O1 Rebecca Vismara - *The role of pore plasticity during benzene/cyclohexane separation in Zr(IV) aromatic-based MOPs and MOFs*

15:50-16:10 O2 Tommaso Battiston - *P-induced crystal-fluid interactions in erionite-K: a natural nano-sponge*

16:10-16:30 O3 Rossella Arletti - *Amino acids adsorption in mordenite zeolite: the effects of spatial confinement and pressure*

MS8: Structure and Function in synthetic and natural nano and polycrystalline materials

Chairs: Elisa Boanini (Università di Bologna), Arianna Lanza (ELDICO Scientific – Villigen - CH)

Invited talks:

14:30-15:00 KN1 Linda Pastero, Università di Torino

Bulk vs surface structure in biological apatites

15:00-15:30 KN2 Andrew Kentaro Inge, University of Stockholm

Green and stable metal-organic frameworks inspired by metallodrugs

Oral presentations:

15:30-15:50 O1 Anna Vivani - *Synthesis and Characterization of Novel Environmentally Sustainable FASnI₃ Perovskite Nanocrystals*

15:50-16:10 O2 Stefano Pasini - *Optimization of the window layers in Sb₂Se₃ thin-film solar cells*

16:10-16:30 O3 Nicole Balasco - *Atomic-Level Three-Dimensional Models of Amyloid-Like Self-Assembling Peptides Derived by Molecular Dynamics*

17:00-18:00 Plenary lecture [Chair: Massimo Degano (IRCCS Scientific Institute San Raffaele)]

Andrea Musacchio, MPI Dortmund (Germany)

The kinetochore: an intrinsically divisive molecular machine

Wednesday 8th September

MS9: Cristallografia, comunicazione scientifica e società

Chairs: Chiara Massera (Università di Parma), Pietro Roversi (CNR - Milano)

Invited talks:

9:00-9:30 KN1 Ilaria Gimondi

Using Crystallography in Education and Outreach – insights from the CCDC

9:30-10:00 KN2 Leonardo Feletto

How COVID-19 spiked the interest for structural biology

10:00-10:30 KN3 Chiara Ceci

Seeing things under a different light: reflections and case studies on communication of crystallography from the United Kingdom

10:30-11:00 Premi “progetti di divulgazione delle scienze cristallografiche” 2020/2021

Francesco Bonì - *Cristalli a Raggi X, dalla malattia alla cura. Presenta Gabriele Princiotta*

Paolo Pio Mazzeo - *GCI talks to... Presenta Marta Morana*

Marzia dell’Aera - *CrystalMApp*

Maria Romano - *Cristallograficamente*

Luigi Scietti - *Cosa è la cristallografia e cosa ha fatto/può fare per voi?*

11:30-12:30 Plenary lecture [Chair: Andrea Ienco (CNR-ICCOM), Sabrina Nazzareni (Università di Perugia)]

Andrea Plazzi, Symmaceo Communications

What we talk about when we talk about Comics&Science

Thursday 9th September

08:30-9:20 Registration

9:20-9:45 Welcome Address

Angela Altomare, Presidente AIC

Paolo Martelli, Prorettore Vicario

Andrea Zappettini, Direttore IMEM-CNR

Roberto Corradini, Direttore Dipartimento SCVSA

09:45-10:30 Mammi Award

Chair: Angela Altomare (IC-CNR Bari)

Martino Bolognesi, Università di Milano

Protein Crystallography Evolution: a Professional Life-Time Experiment

10:30-11:00 Coffe break

11:00-11:20 Nardelli Award 2020

Chair: Carlo Mealli (CNR-ICCOM, Firenze)

Simone d'Agostino, Università degli Studi di Bologna

Crystal Engineering: Harnessing Intermolecular Interactions for the Design of New Materials

11:20-11:40 Nardelli Award 2021

Chair: Carlo Mealli (CNR-ICCOM, Firenze)

Carlotta Giacobbe, ESRF, Grenoble

Crystallography of asbestos fibers. Challenges and (structural) solutions

11:45-12:00 Best PhD Thesis Award 2020

Gabriele Cerutti

Crystal structure and functional characterization of an oligosaccharide dehydrogenase from Pycnoporus cinnabarinus provides insights into fungal breakdown of lignocellulose

12:00-12:15 Best PhD Thesis Award 2020

Rebecca Scatena

Charge and Spin Density based Properties of Materials

12:15-12:30 Best PhD Thesis Award 2021

Ilaria Silvestri

Pioneering strategies for the schistosomiasis treatment by means of a structure-based drug discovery approach

12:35-12:40 Best Graduate Award 2020

Francesco Pagliaro

Crystal-fluid interaction in MFI zeolites at high pressure

12:40-12:45 Best Graduate Award 2021

Pia Antonietta Antignani

Crystallographic orientations and timing relationships of clinopyroxene inclusions in diamond

13:00-15:00 Lunch

15:00-18:30 AIC General Assembly

MS1-O1 High-pressure behavior and crystal chemistry of natural REE-bearing arsenates and phosphates

Francesco Pagliaro^a, Paolo Lotti^a, Davide Comboni^b, Tommaso Battiston^a, Alessandro Guastoni^c, G. Diego Gatta^a, Nicola Rotiroti^a

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^cDipartimento di Geoscienze, Università degli Studi di Padova, Padova, Italy

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Rare Earth Elements (REE) are a group of 17 elements, containing the lanthanides and their geochemical cognates Sc and Y. REEs are fundamental elements in several high-tech applications, including magnets, catalysis and glass additives. All the REEs have been classified as critical raw materials, for their elevated supply risk. Despite their high economic relevance, only few studies have been devoted to the crystal chemistry, behavior and phase stability at non-ambient conditions of natural REE-bearing minerals, characterized by a multi-REE composition. The REE-composition seems to highly influence the stability field of REE-bearing compounds [1] and, in this light, we aim to study the high-*P* phase stability and elastic behavior of four natural multi-REE-bearing minerals, occurring at the Mt. Cervandone deposit (Piedmont, Italy): chernovite-(Y), (nominally $YAsO_4$), gasparite-(Ce) (nominally $CeAsO_4$), xenotime-(Y) (nominally YPO_4) and monazite-(Ce) (nominally $CePO_4$). Chernovite-(Y) and xenotime-(Y) share the same zircon-type structure with tetragonal symmetry (space group $I4_1/amd$) and are characterized by *HREE*- (Gd-Lu series) and Y-enrichment. Conversely, gasparite-(Ce) and monazite-(Ce) share the same *LREE* (La-Eu) enrichment and the so-called monazite-type structure (space group $P2_1/n$). All the selected minerals have been investigated over 20 GPa, using a diamond anvil cell (DAC), by means of in situ synchrotron single-crystal X-ray diffraction. For both the zircon-type structure minerals, a *P*-induced phase transition has been observed: chernovite-(Y) undergoes a transition to a scheelite-type structure at ~11 GPa, as previously observed for its synthetic pure analogue $YAsO_4$ [2]. The phase transition in xenotime-(Y) to a monazite-type structure, as for synthetic pure YPO_4 , is observed between 17 and 19 GPa [3]. However, synthetic YPO_4 is characterized by a second phase transition to a scheelite-type structure [3], but in our natural studied sample a similar behavior has not been observed at least up to 30 GPa. Conversely, for gasparite-(Ce) and monazite-(Ce), no phase transitions occur within the pressure-range under investigation. For all the investigated REE-bearing minerals, both with tetragonal and monoclinic symmetry, the bulk compression is mainly accommodated by the REE-coordination polyhedra. Whereas in the tetragonal chernovite-(Y) and xenotime-(Y) the [001]-axis is the less compressible direction, due to the polyhedral chains running along this axis, in gasparite-(Ce) and monazite-(Ce) the distortion of the $REEO_9$ polyhedra leads to the lowest linear compression laying in the (010) plane and, therefore, not coinciding with the direction of chain development. The structural analysis also reveals that the arsenates are more compressible with respect to the isostructural phosphates. The observed difference in compressibility between phosphates and arsenates is related to the different behavior of the As and P coordination tetrahedra: AsO_4 shows a significant compression, especially in the low-*P* regime, whereas PO_4 substantially behaves as a rigid body under pressure.

[1] Lacomba-Perales, R., Errandonea, D., Meng, Y., & Bettinelli, M. *Phys. Rev.* **2010** *B81*, 064113.

[2] Errandonea, D., Kumar, R., Lopez-Solano, J., Rodriguez-Hernandez, P., Muñoz, A., Rabie, M. G., & Puche, R. S. *Phys. Rev.* **2011** *B83*, 134109.

[3] Zhang, F. X., Wang, J. W., Lang, M., Zhang, J. M., Ewing, R. C., & Boatner, L. A. *Phys. Rev.* **2009** *B80*, 184114.