



5th Meeting
Bologna 5-8 September 2023

Programme

San Giovanni in Monte- Università di Bologna

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ALMA MATER STUDIORUM
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DIPARTIMENTO DI
FARMACIA E BIOTECNOLOGIE

Tuesday 5 September
Aula Prodi- Università di Bologna

- Registration: 13.00-14.45
- Opening
Remarks: 14.45-15.00
Angela Altomare *President AIC*
Elisa Boanini, Lucia Maini *Co-chair congress*
- Plenary
lecture 1: 15.00-15.45
Carmelo Giacobuzzo
IC- CNR, Bari
Get the phase: a century old problem
- Mammi Prize: 15.45-16.30
Alessandro F. Gualtieri
University of Modena and Reggio Emilia
The aid of crystallography to address health and environmental issues caused by mineral fibres
- Nardelli Prize: 16.30-17.00
Stefano Canossa
Max Planck Institute for Solid State Research, Stuttgart
Beyond the average: a journey to the multiscale diversity of framework materials
- Nardelli Prize: 17.00-17.30
Davide Comboni
Università degli Studi di Milano
Phase transition and crystal structure evolution of hydrated borates at high pressure
- Best PhD thesis: 17.30-17.45
Riccardo Fantini
University of Modena and Reggio Emilia
Zeolites as a scaffold for UV filters: from sunscreens to crystallography
- Best PhD thesis: 17.45-18.00
Mattia Lopresti
Università of the Eastern Piedmont "Amedeo Avogadro"
Differential scanning diffraction for in situ investigations of choline-based deep eutectic solvents
- Best master
thesis: 18.00-18.15
Alice Taddei
University of Florence
Thallium incorporation in hydroxychlorite crystals
- Laura Contini**
University of Bologna
Stimuli Responsive Hybrid Coordination Polymers based on Copper Iodide as luminescent mechanochromic materials
- Sofia De Felice**
Università degli Studi di Padova
Structural investigation of *Pseudomonas aeruginosa* SOS machinery components by cryo-EM
- Welcome party 18.15-20.00

Wednesday 6 September - morning
Aula Prodi

Plenary
lecture 2: 9.00-9.45
Dario Braga
Department of Chemistry "Giacomo Ciamician", University of Bologna
A journey in crystal engineering land

Sponsor
presentation : 9.45-10.00
Fraser White
Assing- Rigaku
Rigaku Oxford Diffraction: X-rays, Electrons and more

Coffee break: 10.00-10.30

Parallel
sessions: 10.30-12.30

MS1 Aula Prodi	MS2 Aula Capitani
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Lunch: 12.30-14.00

MS1 - Tailoring noncovalent interactions to design organic crystals

Chairs: P. Metrangolo (Polytechnic University of Milan); P. Paoli (University of Florence)

Keynote 1: 10.30-11.00
Alessia Bacchi
Department of Chemical Sciences, Life Sciences and Environmental Sustainability, University of Parma
Tweaking interactions to achieve release performances in co-crystals

Keynote 2: 11.00-11.30
Chilla Malla Reddy
Department of Chemical Sciences, Indian Institute of Science Education and Research, Kolkata
Crystal engineering of adaptive smart materials

Oral 1: 11.30-11.45
Giovanni Macetti
Department of Chemistry, Università di Milano
Symmetry-constrained Monte Carlo to predict the experimental crystal structure of small organic molecules

Oral 2: 11.45-12.00
Enrico Spoletti
Department of Chemical Science & Bernal Institute, University of Limerick
True Polymorphism in a Solid Solution of Tolbutamide and Chlorpropamide affords a High-Soluble Co-Drug Form

Oral 3: 12.00-12.15
Giovanni Pierri
Department of Chemistry and Biology, University of Salerno
The influence of weak interactions in the backbone conformation and solid state behavior of cyclic peptoids

Oral 4: 12.15-12.30
Luigi Renzo Nassimbeni
Department of Chemistry, University of Cape Town
A survey of Inclusion Compounds: Structure, Selectivity and Kinetics

MS2 - Combined structural methodologies to address complex biological systems

Chairs: M. Milani (IBF-CNR, Milan); L. Cendron (University of Padua)

- Keynote 1: 10.30-10.55
Matteo De Rosa
Institute of Biophysics-CNR
Structural bases of gelsolin-related diseases
- Keynote 2: 10.55-11.20
Alessandra Magistrato
CNR-IOM
Unraveling the molecular mechanism of pre-mRNA splicing via all-atom simulations
- Oral 1: 11.20-11.32
Francesco Rinaldi
Istituto Italiano di Tecnologia
Elucidating the RAD52 architecture through an integrated structural biology approach
- Oral 2: 11.32-11.44
Elisa Fagnani
Department of Biosciences, University of Milano
Understanding the pro-survival role of AIF: structural and functional study of AIF-CHCHD4 complex
- Oral 3: 11.44-12.06
Silvia Garavaglia
Dipartimento di Scienze del Farmaco, University of Piemonte Orientale
Using rational structural analysis for development drugs and diagnostics tools to selective targeting human ALDH1A3 in solid tumours
- Oral 4: 12.06-12.18
Filippo Vascon
Department of Biology, University of Padova
Structural studies on the bacterial SOS response: how it is shaped and how to suppress it
- Oral 5: 12.18-12.30
Sarita Sarita
Department of Biosciences, University of Milano
Structural and molecular features of native and fibril form of AL55 light chain protein associated with AL amyloidosis

Wednesday 6 September - afternoon Aula Prodi

Plenary
lecture 3: 14.00-14.45
Giovanna Scapin
CSO NanoImaging Services
Structural Biology in Drug Discovery

Sponsor
presentation : 14.45-15.00
Eugenio Casini
MalvernPanalytical
Characterization of a few AIBIIXO₄ compounds using both the compact Aeris and the Empyrean platforms

Parallel
sessions: 15.00-17.00

MS3 Aula Capitani

MS4 Aula Prodi

Coffee break: 17.00-17.30

AIC assembly: 17.00-19.00

MS3 - Growth of crystalline functional materials and thin films

Chairs: A. Sassella (University of Milano-Bicocca); S. Rubini (CNR-IOM)

Keynote 1: 15.00-15.30
Cristiano Albonetti
CNR-Istituto per lo Studio dei Materiali Nanostrutturati, Bologna
Identification of ultra-thin molecular layers atop monolayer terraces in sub-monolayer organic films with scanning probe microscopy

Keynote 2: 15.30-16.00
Pasquale Orgiani
CNR-Istituto Officina dei Materiali, Trieste
Crafting the structure of materials for tailoring their quantum properties: the case of anatase TiO₂ thin films

Oral 1: 16.00-16.20
Lucia Maini
Dipartimento di Chimica "G. Ciamician", Università di Bologna
Annealing and deposition procedures to access elusive polymorphs of NDI-C6 in thin film

Oral 2: 16.20-16.40
Eugenia Pechkova
Department of Experimental Medicine, University of Genova
Protein Langmuir-Blodgett Thin Films for Protein Crystallization and Structural Studies

Oral 3: 16.40-17.00
Valentina Zannier
CNR Istituto Nanoscienze and Scuola Normale Superiore, Pisa
Free-standing InSb nanostructures: growth, morphology control and electrical characterization

MS4 - Structural approaches to disclosing molecular recognition and targeting

Chairs: A. Ilari (*Institute of molecular biology and pathology-CNR*); F. Sica (*University of Naples Federico II*)

- Keynote 1: 15.00-15.24
Giuseppina De Simone
CNR-Institute of Biostructures and Bioimaging, Napoli
Carbonic Anhydrase IX as target for the design of novel anticancer drugs: an integrated biochemical, structural, and computational approach
- Keynote 2: 15.24-15.48
Francesco Angelucci
Department of Life, Health and Environmental Sciences, Università degli Studi dell'Aquila
Circumventing nucleophilic active sites of thioredoxin reductases for selective inhibition
- Oral 1: 15.48-16.00
Benny Danilo Belviso
CNR-Istituto di Cristallografia, Bari
Unveiling the structural effects of copper and zinc ions on K48-linked diubiquitin
- Oral 2: 16.00-16.12
Eloise Mastrangelo
Department of Biosciences, University of Milano – CNR-Biophysics Institute
Retromer stabilization for Neuroprotection in Amyotrophic Lateral Sclerosis: analysis of the possible binding sites of bis-1,3-phenyl guanylylhydrazones to the retromer VPS29/VPS35 interface
- Oral 3: 16.12-16.24
Cecilia Pozzi
Department of Biotechnologym Chemistry and Pharmacy, University of Siena
Structural evidence of the dimerization of C-type lectin-like receptor CD93, promoting its binding to Multimerin-2 in endothelial cells
- Oral 4: 16.24-16.36
Alessia Ruggiero
CNR-Institute of Biostructures and Bioimaging, Napoli
Thermotoga maritima Arginine Binding Protein as a model system for understanding protein self- and hetero-interactions
- Oral 5: 16.36-16.48
Carmelinda Savino
CNR-Institute of Molecular Biology and Pathology
Novel insights into fungal catabolism of lignocellulose: structural characterization of an auxiliary enzyme that assists laccase-mediated oxidations
- Oral 6: 16.48-17.00
Ilaria Silvestri
Istituto Italiano di Tecnologia- IC-CNR
Targeting the conserved active site of splicing machines with specific and selective small molecule modulators

Thursday 7 September – morning
Aula Prodi

Plenary
lecture 4: 9.00-9.45
Jacopo Perego
Department of Materials Science, University of Milano Bicocca
Rotors, motors and luminescent properties in metal organic frameworks

Sponsor
presentation : 9.45-10.00
Anna Luebben
Bruker
D8 Venture – collecting better home-lab data

Coffee break: 10.00-10.30

Parallel
sessions: 10.30-12.30

MS5 Aula Capitani

MS6 Aula Prodi

Lunch: 12.30-14.00

MS5 - Challenging 3D structure: equipment, methodologies, and computing

Chairs: D. Siliqi (institute of Crystallography-CNR); A. Rosato (University of Florence)

Keynote 1: 10.30-11.00
Enrico Ravera
University of Florence
Integration in Structural Biology

Keynote 2: 11.00-11.30
Corrado Cuocci
CNR-Istituto di Cristallografia, Bari
Challenging structure solution of microcrystalline materials by the direct space approach in action using the EXPO software

Oral 1: 11.30-11.45
Marco Mazzorana
Diamond Light Source, Oxford
Dose-aware data collection at MX beamlines

Oral 2: 11.45-12.00
Marco Milanesio
University of Piemonte Orientale
Are modern lab powder diffractometers “small large scale facilities”?

Oral 3: 12.00-12.15
Linda Cerofolini
University of Florence
Application of SSNMR for Epitope Mapping and Binding Assessment of multispecific biologics

Oral 4: 12.15-12.30
Danilo Marchetti
University of Parma and Istituto Italiano di Tecnologia
Combined application of 3D electron diffraction analysis and mechanochemical synthesis to identify novel nanocrystalline reticular materials

MS6 - Understanding materials properties through in situ non-ambient and in operando studies

Chairs: P. Lotti (University of Milan); M. Milanesio (University of Eastern Piedmont)

- Keynote 1: 10.30-11.00
Georgia Cametti
University of Bern
Tracking in situ the structural transformations occurring in zeolite as a function of temperature
- Keynote 2: 11.00-11.30
Heinz Amenitsch
Graz University of Technology
Operando Small Angle X-ray Scattering as a tool in energy research
- Oral 1: 11.30-11.45
Andrea Bernasconi
Dipartimento di Scienze della Terra, University of Torino
Structure of Na₂O-CaO-Al₂O₃-SiO₂ glass by *in-situ* total scattering synchrotron experiments
- Oral 2: 11.45-12.00
Paolo P. Mazzeo
University of Parma
Time Resolved In Situ (TRIS) monitoring by X-ray Powder Diffraction of Mechanochemical reactions: a chronical of impacts
- Oral 3: 12.00-12.15
Gianfranco Ulian
Department of Biological, Geological and Environmental Sciences, University of Bologna
Elastic and thermodynamic properties of hydroxylapatite and carbonated apatite from theoretical *ab initio* simulations
- Oral 4: 12.15-12.30
Rebecca Vismara
University of Granada and Universita' dell'Insubria
HR-PXRD isotherms: a tool to understand CO₂ adsorption in an iron(III) pyrazolate MOF

Thursday 7 September – afternoon

Aula Prodi

- Plenary
lecture 5: 14.00-14.45
Ute Kolb
Department of Chemistry, Johannes Gutenberg-University Mainz
3D Electron diffraction (3DED) the ultimate tool for structure analysis from nano crystal?

MS7 - Giovani Cristallografi Italiani

Chairs: R. Vismara (University of Granada); G. Pierri (University of Salerno)

- AIC- GCI
dissemination: 14.45-14.55
Marzia Dell'Aera
Department of Chemistry, University of Zurich
An overview on CrystalMApp
- Oral 1: 14.55-15.10
Vincentia Emerson Agbemeh
Istituto Italiano di Tecnologia
Organic Cocrystals Structures Solved Using 3D Electron Diffraction

- Oral 2: 15.10-15.25
Tommaso Battiston
Department of Earth Sciences, University of Milano
 P-mediated crystal-fluid interaction in the ABC-6 zeolite group: the case of ERI, OFF and EAB topologies
- Oral 3: 15.25-15.40
Martina Lippi
Department of Industrial Engineering, University of Florence
 Further insights into (S)-(+)-naproxen diastereomeric salt formation from ongoing solid state
- Oral 4: 15.40-15.55
Giacomo Montanari
Department of Philosophy and Communication Studies, University of Bologna
 Vitriols: The Many Colors of Iron
- Oral 5: 15.55-16.10
Samet Ocak
Department of Chemistry, University of Bologna
 Exploring the Plastic Phase Transition Characteristics of Quinuclidinium Salts with Diverse Counter-Anions and Their Solid Solutions
- Oral 6: 16.10-16.25
Luca Sironi
Department of Chemistry, University of Milano
 Study of molecular recognition of supercooled benzoic acid with MiCMoS
- Flash 1: 16.25-16.30
Laura Macchietti
Department of Chemistry, University of Bologna
 Application of multivariate analysis on powder diffraction data for the monitoring of a mechanochemical synthesis
- Flash 2: 16.30-16.35
Michele Prencipe
Department of Chemistry, Life Sciences and Environmental Sustainability, University of Parma
 Solid state transformations: a mighty approach through mechanochemistry
- Flash 3: 16.35-16.40
Giusy Tassone
Department of Biotechnology, Chemistry and Pharmacy, University of Siena
 Evidence of amino-thiadiazoles as innovative inhibitors of human glutaminyl cyclase, validated target for neurodegenerative disorders
- Flash 4: 16.40-16.45
Gabriella Tito
Department of Chemical Sciences, University of Naples Federico II
 Structural characterization of the adduct formed upon reaction of dirhodium tetraacetate with a double helix dodecamer
- Coffee break: 16.45-17.00
- Poster session with aperitive: 17.00-19.00
- Social dinner: 20.30
Ristorante Biagi- Via Saragozza, 65a, 40123 Bologna BO

Friday 8 September – morning
Aula Prodi

Plenary
lecture 6: 9.00-9.45
Michele Zema
Department of Earth and Geo-environmental Sciences
The growing community of crystallographers

Sponsor
presentation : 9.45-10.00
Andrew Jones
Anton Paar
Latest advances in powder XRD instrumentation

Coffee break: 10.00-10.30

Parallel
sessions: 10.30-12.30

MS8 Aula Prodi	MS9 Aula Capitani
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Final remarks: 12.30-13.00

MS8 - Mineralogy: recent developments and applications

Chairs: P. Ballirano (Sapienza University of Rome); P. Comodi (University of Perugia)

Keynote 1: 10.30-11.00
Fabrizio Bardelli
CNR-Istituto di Nanotecnologia, Roma
Combining X-ray diffraction and X-ray absorption spectroscopy to study Asbestos Bodies in human lung tissues

Keynote 2: 11.00-11.30
Rossella Arletti
Department of Chemical and Geological Sciences, University of Modena and Reggio Emilia
Secondary and alternative raw materials for ceramic tile production: a mineralogical point of view

Oral 1: 11.30-11.45
Lisa Baratelli
Department of Earth Sciences, University of Milano
Crystal-chemistry and polytypism in lombardoite, Ba₂Mn(AsO₄)₂(OH)

Oral 2: 11.45-12.00
Ferdinando Bosi
Department of Earth Sciences, Sapienza University of Rome
On the endmember composition

Oral 3: 12.00-12.15
Andrea Bisciotti
Department of Physics and Earth Sciences, University of Ferrara
Rietveld QPA for imaging calibration and to predict engineering properties in recycling of construction and demolition waste

Oral 4: 12.15-12.30
Serena C. Tarantino
Department of Chemistry, University of Pavia
Transforming Biosolid Waste into Secondary Raw Materials for Sustainable Materials Production

MS9 - Structural aspects of metal-based systems for the sustainable development

Chairs: V. Colombo (University of Milan); L. Marchiò (University of Parma)

- Keynote 1: 10.30-11.00
Elisa Borfecchia
Department of Chemistry, University of Torino
Understanding local structure and reactivity of copper-based catalysts for the valorization of light alkanes: from Cu-zeolites to Cu-MOFs
- Keynote 2: 11.00-11.30
Lorenzo Malavasi
Department of Chemistry, University of Pavia
Structure-property correlations in metal halide perovskites: a route to design optimized and novel materials for energy applications
- Oral 1: 11.30-11.45
Mauro Coduri
Department of Chemistry, University of Pavia
Beyond entropy: understanding the phase stability of high entropy oxide $Mg_{0.2}Co_{0.2}Ni_{0.2}Cu_{0.2}Zn_{0.2}O$
- Oral 2: 11.45-12.00
Andrea Daolio
Department of Materials Science, University of Milano
Dipolar molecular rotors in fluorinated MOFs and CO₂ capture
- Oral 3: 12.00-12.15
Dario Giovanardi
Department of Chemical Sciences, Life Sciences and Environmental Sustainability, University of Parma
From Essential Oils to Active Food Packaging: two ML-MOFs compared
- Oral 4: 12.15-12.30
Simona Galli
Università dell'Insubria
Mercury sequestration-driven phase transition of a luminescent Zn-MOF: a multi-technique study



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