

*Program*  
**4th Joint AIC - SILS  
Conference**



**TRIESTE, 12-15 SEPTEMBER 2022**

# 4<sup>th</sup> Joint AIC-SILS Conference – Trieste, 12-15 September 2022

## COMMITTEES

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### Steering Committee

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## 4<sup>th</sup> Joint AIC-SILS Conference – Trieste, 12-15 September 2022

### Under the Patronage of:



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## ***Conference Schedule***

# 4<sup>th</sup> Joint AIC-SILS Conference



Trieste September 12-15 2022

Monday 12<sup>th</sup> September 2022

<b>Registration</b>		
Parco di San Giovanni - Building N - Meeting Room	12:00 - 13:45	
<b>Conference Open Cerimony</b>		
Parco di San Giovanni - Teatrino Franco Basaglia	14:00 - 14:30	<b>Chairs:</b> Francesco Princivalle - University of Trieste, Silvano Geremia - University of Trieste
Roberto Di Lenarda - University of Trieste - <b>Dean</b> Angela Altomare - Institute of Crystallography CNR, Bari - <b>President AIC - Conference Chair</b> Cinzia Giannini - Institute of Crystallography CNR, Bari - <b>President SILS - Conference Chair</b> Federico Boscherini - University of Bologna - <b>Chair of the Conference Scientific Committee</b> Dorian Lamba - Institute of Crystallography CNR, Trieste - <b>Chair of the Conference Organizing Committee</b>		
<b>Plenary Lecture</b>		
PL-1 - Sharon Shwartz - Bar-Ilan University, Ramat-Gan - ISR	14:30 - 15:30	<b>Chair:</b> Cinzia Giannini - Institute of Crystallography CNR, Bari - <b>President SILS</b> Quantum imaging with X-rays
<b>Coffee Break</b>		
	15:30 - 16:00	
<b>Awarding AIC - SILS Prizes</b>		
		<b>Chairs:</b> Angela Altomare - Institute of Crystallography CNR, Bari - <b>President AIC</b> , Cinzia Giannini - Institute of Crystallography CNR, Bari - <b>President SILS</b>
<b>AIC - "Mario Nardelli" Prize ex-aequo</b>		
<b>Award Ceremony</b>		
Paolo Pio Mazzeo - University of Parma	16:00 - 16:05	
	16:05 - 16:25	Crystal Engineering for storage and release of molecular active ingredients
Marco Taddei - University of Pisa	16:25 - 16:45	The quest for ordered porosity in zirconium phosphonates: blood, sweat and tears (and powder X-ray diffraction)
<b>Best PhD Thesis - "Fiorenzo Mazzi" Prizes</b>		
<b>Award Ceremony</b>		
Rosaria Bruno - University of Calabria	16:45 - 16:50	
	16:50 - 17:00	Metal-Organic Frameworks as advanced porous materials for gas separation and water remediation.
Alessandro Grinzato - University of Padova	17:00 - 17:10	Applications of Cryo-Electron Microscopy in Structural Biology
Daniela Mauro - University of Pisa	17:10 - 17:20	Crystal-chemistry of the secondary minerals of the thallium-rich pyrite ores from the Apuan Alps (Tuscany, Italy)
<b>Best BAMS Thesis - "Fiorenzo Mazzi" Prizes</b>		
<b>Certificate Delivery Ceremony</b>		
Lisa Baratelli - University of Milano	17:20 - 17:25	
	17:25 - 17:30	Crystal chemical study of arsenates and vanadates of the brackebuschite supergroup from Valletta mine, Canosio, Val Maira (CN)
Tommaso Battiston - University of Milano	17:30 - 17:35	Thermal and compressional behavior of the natural borate kurnakovite, (MgB <sub>2</sub> O <sub>4</sub> (OH) <sub>5</sub> ·5H <sub>2</sub> O)
Luca Sironi - University of Milano	17:35 - 17:40	Combined Experimental and Computational Studies on Molecular Recognition among D-Glucose Molecules
<b>SILS - Young Scientist Prize</b>		
<b>Award Ceremony</b>		
Alberta Terzi - Institute of Crystallography CNR, Bari	17:40 - 17:45	
	17:45 - 18:05	The health seen through collagen network: from disease to regeneration
<b>SILS - PhD Thesis "Carlo Lamberti" Prize</b>		
<b>Award Ceremony</b>		
Mariela Romano - Ludwig Maximilian University, München - DE	18:05 - 18:10	
	18:10 - 18:20	A multi-technique hierarchical X-ray phase-based approach for the characterization and quantification of the effects of novel radiotherapies
<b>Mineralogy 2022</b>		
Giuseppe Cruciani - University of Ferrara	18:20 - 18:35	<b>Chair:</b> Diego Gatta - University of Milano - <b>Past President AIC</b> "Mineralogy 2022": a worldwide celebration of mineralogy to highlight its importance in our everyday lives
<b>Panel Discussion</b>		
<b>Horizon-Europe and the Future of Research Infrastructures: Next Generation of Scientific Instrumentation, Tools and Methods</b>		<b>Moderator:</b> Alberto Morgante - University of Trieste
Giorgio Rossi - University of Milano	18:35 - 18:45	NFFA-Europe Pilot: An Open Access Nanoscience Laboratory
Giorgio Paolucci - Elettra-Sincrotrone Trieste, Trieste	18:45 - 18:55	ELETTRA & Fermi Light Sources: status and upgrades
Ornela De Giacomo - Central European Infrastructure Consortium - ERIC, Trieste	18:55 - 19:05	CERIC-ERIC: A Multidisciplinary Research Infrastructure
Alberto Morgante - University of Trieste	19:05 - 19:15	National Research Infrastructure Plan: CNR@Elettra2.0
<b>Questions Time</b>		
	19:15 - 19:20	
<b>Meeting - AIC Biological Macromolecules Group</b>		
Dip. di Matematica e Geoscienze Building O - Lecture Hall A Parco San Giovanni		19:20 - 20:00
<b>Meeting - AIC Young Crystallographers Group</b>		
Dip. di Matematica e Geoscienze Building O - Lecture Hall B Parco San Giovanni		
<b>Welcome Party &amp; Concert of the Ricmanje Orchestra Wind Quintet</b>		
Anfiteatro - Roseto Parco di San Giovanni	20:00 - 21:30	

# 4<sup>th</sup> Joint AIC-SILS Conference



Trieste September 12-15 2022

**Tuesday 13<sup>th</sup> September 2022**

**University of Trieste - Department of Chemical and Pharmaceutical Sciences - Building C11 - Ground Floor - Main Lecture Hall**

**Plenary Lecture**

**Chair: Simona Galli** - University of Insubria, Como  
**PL-2 - Simon Parsons** - University of Edinburgh - UK 08:45 - 09:45 High pressure phase transitions in molecular crystals

**Coffee Break - Building C11 - Ground Floor - Atrium** 09:45 - 10:15

**University of Trieste - Department of Chemical and Pharmaceutical Sciences - Building C11 - III Floor - Lecture Hall A1**

**MS-01 Modern Integrative Structural Biology**

**Chairs: Stefano Mangani** - University of Siena, **Beatrice Vallone** - University of Roma "La Sapienza", Roma

KNL-1 <b>Marina Mapelli</b> - European Institute of Oncology, Milano	10:15 - 10:45	Molecular crosstalk between fate determination and orientation in epithelial cell divisions
KNL-2 <b>Antonio Chaves-Sanjuan</b> - University of Milano	10:45 - 11:15	Structural characterization of a post-mortem amyloid fibril from a cat kidney
O-1 <b>Sonia Covaceuszach</b> - Institute of Crystallography CNR, Trieste	11:15 - 11:30	Insights on the structural determinants of proBDNF V66M variant, a modifier in neuropsychiatric disorders severity
O-2 <b>Benny Danilo Belviso</b> - Institute of Crystallography CNR, Bari	11:30 - 11:45	C-terminus of the histone-lysine N-methyltransferase NSD3 characterized by small-angle X-ray scattering
O-3 <b>Emiliano De Santis</b> - University of Uppsala - SE	11:45 - 12:00	Directional explosion. A hybrid simulation study
F-1 <b>Cecilia Pozzi</b> - University of Siena	12:00 - 12:05	Structural insights into the hYAP-hTEAD4 protein-protein interaction: an emerging target in cancer treatment
F-2 <b>Roberto Marotta</b> - Italian Institute of Technology, Genova	12:05 - 12:10	Unravelling the regulation pathway of photosynthetic AB-GAPDH
F-3 <b>Francesca Paoletti</b> - National Chemistry Institute, Ljubljana - SLO	12:10 - 12:15	Landscape of the ATP binding to neurotrophins: effects on conformation and dynamic modulation by divalent cations

**Commercial Presentations Session I - Building C11 - III Floor - Lecture Hall A1**

**Chair: Alberto Cassetta** - Institute of Crystallography CNR, Trieste

S-1 <b>Andrea Pigozzo</b> - Alfatest Srl, Roma	12:15 - 12:45	Pushing the boundaries in biomolecular stability and interaction analysis with GCI and MicroCal
S-2 <b>Max Maletta</b> - Thermo Fisher Scientific, Eindhoven - NL	12:45 - 13:15	Peeping into the cell with Cryo-Electron Tomography

**e-Poster Session I & Commercial Exhibit I - Building C11 - III Floor - Atrium** 12:15 - 13:15

**Buffet Lunch - Building C11 - Ground Floor - Atrium** 13:15 - 14:15

**University of Trieste - Department of Chemical and Pharmaceutical Sciences - Building C11 - III Floor - Lecture Hall A1**

**MS-04 Frontiers in Mineralogy and Inorganic Geochemistry**

**Chairs: Donato Belmonte** - University of Genova, **Gabriele Giuli** - University of Camerino

KNL-1 <b>Paolo Lotti</b> - University of Milano	14:30 - 15:00	Crystal chemistry of natural REE-phosphates and arsenates and their (T,P)-behavior
KNL-2 <b>Nicola Campomenosi</b> - University of Hamburg - DE	15:00 - 15:29	Elastic vs. visco-plastic rheology of stressed host-inclusion mineral systems at non-ambient conditions: insights from in situ Raman spectroscopy
O-1 <b>Mattia La Fortezza</b> - University of Genova	15:29 - 15:43	Ab initio thermodynamics of MgSiO <sub>3</sub> protoenstatite at high temperatures conditions
O-3 <b>Sabrina Nazzareni</b> - University of Perugia	15:43 - 15:57	High pressure single-crystal synchrotron XR diffraction of natural pyrochlores
O-2 <b>Simone Pollastri</b> - Elettra-Sincrotrone Trieste, Trieste	15:57 - 16:11	Characterization of bottom ashes from incineration process by means of XRF mapping and XANES spectroscopy
O-4 <b>Sirio Consani</b> - University of Pisa	16:11 - 16:25	The Cu-Fe-Ni-Co sulphide ore deposits of the Monte Ramazzo-Lagoscuro mines
F-1 <b>Francesca Menescardi</b> - University of Genova	16:25 - 16:30	Molecular dynamics strategies to determine the melting curve of CaO

**Coffee Break - Building C11 - Ground Floor - Atrium** 16:30 - 17:00

**ePoster Session II & Commercial Exhibit II - Building C11 - III Floor - Atrium** 17:00 - 18:00

**AIC General Assembly - Building C11 - Ground Floor - Main Lecture Hall** 18:00 - 20:00

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Trieste September 12-15 2022

**Tuesday 13<sup>th</sup> September 2022**

**University of Trieste - Department of Chemical and Pharmaceutical Sciences - Building C11 - Ground Floor - Main Lecture Hall**

**Plenary Lecture**

**Chair: Simona Galli** - University of Insubria, Como

**PL-2 - Simon Parsons** - University of Edinburgh - UK 08:45 - 09:45 High pressure phase transitions in molecular crystals

**Coffee Break - Building C11 - Ground Floor - Atrium** 09:45 - 10:15

**University of Trieste - Department of Chemical and Pharmaceutical Sciences - Building C11 - III Floor - Lecture Hall A2**

**MS-07 Materials at Extreme Conditions: X-ray Crystallography and Beyond**

**Chairs: Giuliana Aquilanti** - Elettra-Sincrotrone Trieste, Trieste, **Davide Comboni** - ESRF, Grenoble - FR

KNL-1 <b>Wilson Crichton</b> - ESRF, Genoble - FR	10:15 - 10:45	Exploring phase diagrams, structures and properties with the large volume press at the ESRF
KNL-2 <b>Boby Joseph</b> - Elettra-Sincrotrone Trieste, Trieste	10:45 - 11:15	Role of crystal lattice in pressure induced electronic transitions : selected examples
O-1 <b>Marta Morana</b> - University of Pavia	11:15 - 11:30	X-ray diffraction shines light on mineral inclusions: a natural high-pressure experiment
O-2 <b>Tommaso Battiston</b> - University of Milano	11:30 - 11:45	P-mediated crystal-fluid interaction in ERI and OFF topology
O-3 <b>Benedetta Chrappan Soldavini</b> - University of Milano	11:45 - 12:00	Structure determination of CaSiO <sub>3</sub> wollastonite polymorphs at HP/HT conditions by single crystal in-situ diffraction
F-1 <b>Maryam Abdolrahimi</b> - University of Roma "Roma Tre", Roma	12:00 - 12:05	Depth selective local coordination in amorphous Co <sub>x</sub> Fe <sub>3</sub> B <sub>2</sub> thin films probed by XAFS under x-ray standing wave condition

**Commercial Presentations Session I - Building C11 - III Floor - Lecture Hall A1**

**Chair: Alberto Cassetta** - Institute of Crystallography CNR, Trieste

S-1 <b>Andrea Pigozzo</b> - Alfatest Srl, Roma	12:15 - 12:45	Pushing the boundaries in biomolecular stability and interaction analysis with GCI and MicroCal
S-2 <b>Max Maletta</b> - Thermo Fisher Scientific, Eindhoven - NL	12:45 - 13:15	Peeping into the cell with Cryo-Electron Tomography

**e-Poster Session I & Commercial Exhibit I - Building C11 - III Floor - Atrium** 12:15 - 13:15

**Buffet Lunch - Building C11 - Ground Floor - Atrium** 13:15 - 14:15

**University of Trieste - Department of Chemical and Pharmaceutical Sciences - Building C11 - III Floor - Lecture Hall A2**

**MS-05 Experimental Design & Analysis of Data**

**Chair: Marco Milanese** - University of University of Eastern Piedmont, Alessandria

KNL-1 <b>Ilaria Carlomagno</b> - Elettra-Sincrotrone Trieste, Trieste	14:30 - 15:00	Combining experimental and statistical tools for an all-round approach to cultural heritage
KNL-2 <b>Dmitry Chernyshov</b> - ESRF, Grenoble - FR	15:00 - 15:30	Synchrotron in situ experimentation, big data, and new tools for fast data processing and analysis
O-1 <b>Nodoka Hara</b> - University of Camerino	15:30 - 15:45	Relativistic effects in EXAFS: overview and application to gold
O-2 <b>Roberta Totani</b> - Institute of Structure of Matter CNR, Trieste	15:45 - 16:00	Spectroscopic investigations of nitroxide persistent organic radicals. Future perspectives in view of Elettra 2.0: the MOST beamline
O-3 <b>Stevan Vrbaski</b> - University of Trieste	16:00 - 16:15	Material density and effective atomic number maps of soft tissues via synchrotron radiation spectral CT
F-1 <b>Mattia Lopresti</b> - University of Eastern Piedmont, Alessandria	16:15 - 16:20	Principal component scores projection on a barycentric coordinate system for a quantification in polycrystalline mixtures XRPD data without crystal structure data
F-2 <b>Gabriele Bonano</b> - University of Modena & Reggio Emilia	16:20 - 16:25	Thin liquid flat-jet for spectroscopy in the soft x-ray photon energy range

**Coffee Break - Building C11 - Ground Floor - Atrium** 16:30 - 17:00

**ePoster Session II & Commercial Exhibit II - Building C11 - III Floor - Atrium** 17:00 - 18:00

**AIC General Assembly - Building C11 - Ground Floor - Main Lecture Hall** 18:00 - 20:00

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Trieste September 12-15 2022

Tuesday 13<sup>th</sup> September 2022

University of Trieste - Department of Chemical and Pharmaceutical Sciences - Building C11 - Ground Floor - Main Lecture Hall

**Plenary Lecture**

**PL-2 - Simon Parsons** - University of Edinburgh - UK | 08:45 - 09:45 | High pressure phase transitions in molecular crystals

**Chair: Simona Galli** - University of Insubria, Como

**Coffee Break - Building C11 - Ground Floor - Atrium** | 09:45 - 10:15

University of Trieste - Department of Chemical and Pharmaceutical Sciences - Building C11 - III Floor - Lecture Hall A3

**MS-03 Italy@EuXFEL**

**Chair: Sakura Pascarelli** - European XFEL, Hamburg - DE

KNL-1 <b>Matteo Pancaldi</b> - Elettra-Sincrotrone Trieste, Trieste	10:15 - 10:45	Megahertz-rate ultrafast X-ray scattering and holographic imaging at the European XFEL
KNL-2 <b>Valerio Cerantola</b> - European XFEL, Hamburg - DE	10:45 - 11:15	Ultra-fast structural dynamics in materials at extreme conditions
O-1 <b>Leonardo Martinelli</b> - Polytechnic University of Milano	11:15 - 11:30	First high energy and temporal resolution pump-probe RIXS at the EuXFEL
O-2 <b>Valerio Bellucci</b> - European XFEL, Hamburg - DE	11:30 - 11:45	Fast 4D X-ray imaging at European XFEL
O-3 <b>Francesco Dallari</b> - DESY, Hamburg - DE	11:45 - 12:00	Microsecond dynamics in complex liquids with MHz XPCS
O-4 <b>Oliviero Cannelli</b> - École Polytechnique Fédérale de Lausanne, Lausanne - CH	12:00 - 12:15	Mapping excitation-specific electron, spin and nuclear dynamics in spinel Co <sub>3</sub> O <sub>4</sub> thin films with femtosecond X-ray emission spectroscopy and diffraction

**Commercial Presentations Session I - Building C11 - III Floor - Lecture Hall A1**

**Chair: Alberto Cassetta** - Institute of Crystallography CNR, Trieste

S-1 <b>Andrea Pigozzo</b> - Alfatest Srl, Roma	12:15 - 12:45	Pushing the boundaries in biomolecular stability and interaction analysis with GCl and MicroCal
S-2 <b>Max Maletta</b> - Thermo Fisher Scientific, Eindhoven - NL	12:45 - 13:15	Peeping into the cell with Cryo-Electron Tomography

**e-Poster Session I & Commercial Exhibit I - Building C11 - III Floor - Atrium** | 12:15 - 13:15

**Buffet Lunch - Building C11 - Ground Floor - Atrium** | 13:15 - 14:15

**Coffee Break - Building C11 - Ground Floor - Atrium** | 16:30 - 17:00

**ePoster Session II & Commercial Exhibit II - Building C11 - III Floor - Atrium** | 17:00 - 18:00

**AIC General Assembly - Building C11 - Ground Floor - Main Lecture Hall** | 18:00 - 20:00



# 4<sup>th</sup> Joint AIC-SILS Conference



Trieste September 12-15 2022

Wednesday 14<sup>th</sup> September 2022

University of Trieste - Department of Chemical and Pharmaceutical Sciences - Building C11 - Ground Floor - Main Lecture Hall

**Plenary Lecture**

**Chair: Paola Prete** - Institute for Microelectronics and Microsystems CNR, Lecce

PL-3 - Heike E. Riel - IBM Research Europe, Rüschlikon - CH 08:45 - 09:45 Nanoscience & Nanotechnology Powering the Digitization of Our World

Coffee Break - Building C11 - Ground Floor - Atrium 09:45 - 10:15

University of Trieste - Department of Chemical and Pharmaceutical Sciences - Building C11 - III Floor - Lecture Hall A1

**MS-06 Crystallographic and Spectroscopic Advanced Tools Applied to Pharmaceuticals** **Chair: Fabia Gozzo** - Excelsus Structural Solutions AG, Villingen - CH

KNL-1 Carmine Talarico - Dompé Farmaceutici SpA, Napoli	10:15 - 10:45	Structural Insights into TRPM Channels. A Long and Unexpected Journey
KNL-2 Arnaud Graudery - Novartis Pharma AG, Basel - CH	10:45 - 11:15	Relevance of solid form's curriculum for drug product development: beyond polymorphism of drug substance
O-1 Matteo Daldosso - Aptuit-Evotec, Verona	11:15 - 11:30	The "Form Selection Process" in the Pharmaceutical Industry: the importance of being Earnest
O-2 Mathilde Reinle-Schmitt - Excelsus Structural Solutions AG, Villingen - CH	11:30 - 11:45	Advances in the quantification of amorphous pharmaceuticals via Multivariate Analysis of Synchrotron X-Ray Powder Diffraction Patterns
O-3 Paola Storici - Elettra-Sincrotrone Trieste, Trieste	11:45 - 12:00	The structural biology task force at Elettra to support drug discovery against Covid-19
F-1 Giusy Tassone - University of Siena	12:00 - 12:05	Structural characterization of human Heat shock protein 90 N-terminal domain in complex with a potent 1,2,3-triazole based inhibitor
F-2 Pietro Delre - Institute of Crystallography CNR, Bari	12:05 - 12:10	Prediction of hERG-Mediated Cardiotoxicity based on the integration of docking scores and protein-ligand interaction fingerprints
F-3 Romualdo Troisi - University of Napoli "Federico II", Napoli	12:10 - 12:15	Unusual binding ability of anticoagulant aptamers revealed by the crystallographic analysis of an engineered pseudo-cyclic TBA in complex with $\alpha$ -thrombin

**Commercial Presentations Session II - Building C11 - III Floor - Lecture Hall A1** **Chair: Alberto Cassetta** - Institute of Crystallography CNR, Trieste

S-1 Hendrik Wuensche - Sartorius, Göttingen - DE 12:15 - 12:45 A biolayer interferometry overview and BLI-MS combination to detect unknown binding partners in crude biological extracts

e-Poster Session III & Commercial Exhibit III - Building C11 - III Floor - Atrium 12:15 - 13:15

Buffet Lunch - Building C11 - Ground Floor - Atrium 13:15 - 14:15

University of Trieste - Department of Chemical and Pharmaceutical Sciences - Building C11 - III Floor - Lecture Hall A1

**MS-09 Current Approaches in Structural Biology** **Chairs: Michele Cianci** - Polytechnic University of Marche, Ancona, **Simona Fermari** - University of Bologna

KNL-1 Rita Berisio - Institute of Biostructures and Bioimaging CNR, Napoli	14:30 - 15:00	X-ray crystallography for vaccine development against emerging pathogens
KNL-2 Mauro Gemmi - Italian Institute of Technology, Pontedera	15:00 - 15:30	3D electron diffraction of beam sensitive samples of biological interest: proteins and pharmaceuticals
O-1 Ida Freda - University of Roma "La Sapienza", Roma	15:30 - 15:45	Single particle cryo-EM unveils multiple states in PdxR mechanism of transcriptional regulation
O-2 Charles J Hitchman - University of Leicester, UK	15:45 - 16:00	Towards the Cryo-EM structure of the ERAD glycoprotein folding checkpoint, the EDEM:PDI heterodimer
O-3 Eloise Mastrangelo - Institute of Biophysics CNR, Milano	16:00 - 16:15	RNA-viruses inhibitors: unintended consequences of the target driven approach
F-1 Serena Rocchio - European Molecular Biology Laboratory, Grenoble - FR	16:15 - 16:20	Fully autonomous end-to-end protein to structure pipelines at MASSIF-1 using the CrystalDirect harvester
F-2 Francesca Rossi - University of Bologna	16:20 - 16:25	Characterization of Ca-depositions evolution by cryo-XANES and cryo-STX in SaOS-2 osteosarcoma cells
F-3 Alberta Terzi - Institute of Crystallography CNR, Bari	16:25 - 16:30	Glycation in collagen macromolecule of diabetic biotissues

Coffee Break - Building C11 - Ground Floor - Atrium 16:30 - 17:00

ePoster Session IV & Commercial Exhibit IV - Building C11 - III Floor - Atrium 17:00 - 18:00

SILS General Assembly - Building C11 - Ground Floor - Main Lecture Hall 18:00 - 20:00

Gala Dinner - Caffè Tommaseo Piazza Nicolò Tommaseo, 4 - Trieste 20:30 - 22:00

# 4<sup>th</sup> Joint AIC-SILS Conference



Trieste September 12-15 2022

Wednesday 14<sup>th</sup> September 2022

University of Trieste - Department of Chemical and Pharmaceutical Sciences - Building C11 - Ground Floor - Main Lecture Hall

## Plenary Lecture

**Chair: Paola Prete** - Institute for Microelectronics and Microsystems CNR, Lecce

PL-3 - Heike E. Riel - IBM Research Europe, Rüschlikon - CH 08:45 - 09:45 Nanoscience & Nanotechnology Powering the Digitization of Our World

Coffee Break - Building C11 - Ground Floor - Atrium 09:45 - 10:15

University of Trieste - Department of Chemical and Pharmaceutical Sciences - Building C11 - III Floor - Lecture Hall A2

## MS-02 Understanding Advanced Functional Materials Through Operando Studies

**Chairs: Elisa Borfecchia** - University of Torino, **Simona Galli** - University of Insubria, Como

KNL-1 Janis Timoshenko - Fritz Haber Institute, Berlin - DE	10:15 - 10:45	Understanding the structure-properties relationship in nanocatalysts for CO <sub>2</sub> electroreduction using time-resolved XAS and advanced data analysis
KNL-2 Marco Ranocchiaro - Paul Scherrer Institute, Villigen - CH	10:45 - 11:15	Characterization of metal-organic frameworks with synchrotron and neutron sources for catalytic applications
O-1 Mariam Maisuradze - University of Bologna	11:15 - 11:30	Operando and ex-situ PXRD Study of Ni-doped Manganese Hexacyanoferrate Cathode Material in Aqueous Zn-ion Battery System
O-2 Andrea Martini - Fritz Haber Institute, Berlin - DE	11:30 - 11:45	Tracking the evolution of Ni-based single atom catalysts for the CO <sub>2</sub> electroreduction reaction: an operando XAS study assisted by machine learning techniques
O-3 Paolo Pio Mazzeo - University of Parma	11:45 - 12:00	On the mechanism of cocrystal mechanochemical reaction via low melting eutectic: a time resolved in-situ monitoring investigation
F-1 Davide Salusso - University of Torino	12:00 - 12:05	MZrO <sub>x</sub> (M = Zn, Ga) catalysts for CO <sub>2</sub> hydrogenation reaction: exploiting XAS and PXRD to understand catalyst's structure, activity and stability
F-2 Martina Lippi - University of Firenze	12:05 - 12:10	Hg(II)-bispidine 1D coordination polymers: three different topologies and their dynamic behavior in solvent adsorption and exchange processes

## Commercial Presentations Session II - Building C11 - III Floor - Lecture Hall A1

**Chair: Alberto Cassetta** - Institute of Crystallography CNR, Trieste

S-1 Hendrik Wuensche - Sartorius, Göttingen - DE 12:15 - 12:45 A biolayer interferometry overview and BLI-MS combination to detect unknown binding partners in crude biological extracts

e-Poster Session III & Commercial Exhibit III - Building C11 - III Floor - Atrium 12:15 - 13:15

Buffet Lunch - Building C11 - Ground Floor - Atrium 13:15 - 14:15

University of Trieste - Department of Chemical and Pharmaceutical Sciences - Building C11 - III Floor - Lecture Hall A2

## MS-10 Investigating Molecular Crystals: Methods and Application

**Chairs: Alessandra Forni** - Institute of Chemical Sciences and Technologies CNR, Milano, **Emanuele Priola** - University of Torino

KNL-1 Alessandro Genoni - CNRS & University of Lorraine, Metz - FR	14:30 - 15:00	Refining structures of molecular crystals through modern methods of quantum crystallography
KNL-2 Domenica Marabello - University of Torino	15:00 - 15:30	From crystallography to physical properties: what the second harmonic generation property is due to?
O-1 Danilo Marchetti - University of Parma	15:30 - 15:45	Dynamic Behaviour of a Tetrapyrroline-Based Crystalline Supramolecular Organic Framework
O-2 Lucia Carlucci - University of Milano	15:45 - 16:00	Porous and luminescent coordination complexes and networks assembled from a new ligand of nanometric length
O-3 Mateja Pisciarić - University of Zagreb - HR	16:00 - 16:15	Shaping crystals using mechanical force: A structural perspective on flexible crystalline coordination polymers of cadmium(II)
F-1 Giovanni Pierri - University of Salerno	16:15 - 16:20	Exploring weak interactions realm with cyclic peptoids
F-2 Michele Prencipe - University of Parma	16:20 - 16:25	Cocrystallization as effective tool for driving the release of natural active compounds
F-3 Elena Simone - Polytechnic University of Torino	16:25 - 16:30	Crystal engineering as a tool for rational design of novel sustainable food, agrochemical and pharmaceutical formulations

Coffee Break - Building C11 - Ground Floor - Atrium 16:30 - 17:00

ePoster Session IV & Commercial Exhibit IV - Building C11 - III Floor - Atrium 17:00 - 18:00

SILS General Assembly - Building C11 - Ground Floor - Main Lecture Hall 18:00 - 20:00

Gala Dinner - Caffè Tommaseo Piazza Nicolò Tommaseo, 4 - Trieste 20:30 - 22:00

# 4<sup>th</sup> Joint AIC-SILS Conference



Trieste September 12-15 2022

Wednesday 14<sup>th</sup> September 2022

University of Trieste - Department of Chemical and Pharmaceutical Sciences - Building C11 - Ground Floor - Main Lecture Hall

## Plenary Lecture

PL-3 - Heike E. Riel - IBM Research Europe, Rüschlikon - CH 08:45 - 09:45 **Chair: Paola Prete** - Institute for Microelectronics and Microsystems CNR, Lecce  
Nanoscience & Nanotechnology Powering the Digitization of Our World

Coffee Break - Building C11 - Ground Floor - Atrium 09:45 - 10:15

University of Trieste - Department of Chemical and Pharmaceutical Sciences - Building C11 - III Floor - Lecture Hall A3

## MS-08 Bright Radiation Sources and Novel Software Applications

**Chairs: Corrado Cuocci** - Institute of Crystallography CNR, Bari, **Francesco Stellato** - University of Roma "Tor Vergata", Roma

KNL-1 Davide Ceresoli - Institute of Chemical Sciences and Technologies CNR, Milano	10:15 - 10:45	Solid State NMR Spectroscopy with Quantum ESPRESSO
KNL-2 Emiliano Principi - Elettra-Sincrotrone Trieste, Trieste	10:45 - 11:15	Ultrafast Light Source Facilities: an Opportunity for Science
O-1 Zeinab Ebrahimpour - National Institute of Nuclear Physics, Frascati	11:15 - 11:30	The EuPRAXIA FEL project: ultra-bright light pulses for imaging and spectroscopy
O-2 Nicola Corriero - Institute of Crystallography CNR, Bari	11:30 - 11:45	A machine learning-based web platform for crystal system classification: CrystalMELA
O-3 Marco Milanese - University of Eastern Piedmont, Alessandria	11:45 - 12:00	PCA analysis of in situ X-ray powder diffraction and imaging data: new approaches named differential scanning diffraction and imaging
F-1 Marco Mazzorana - Diamond Light Source Ltd, Didcot - UK	12:00 - 12:05	Unattended MX data collection and beamline monitoring at Diamond
F-2 Annie Heroux - Elettra-Sincrotrone Trieste, Trieste	12:05 - 12:10	XRD2 to $\mu$ XRD: Italian beamlines dedicated to macromolecular crystallography

## Commercial Presentations Session II - Building C11 - III Floor - Lecture Hall A1

**Chair: Alberto Cassetta** - Institute of Crystallography CNR, Trieste

S-1 Hendrik Wuensche - Sartorius, Göttingen - DE 12:15 - 12:45  
A bilayer interferometry overview and BLI-MS combination to detect unknown binding partners in crude biological extracts

e-Poster Session III & Commercial Exhibit III - Building C11 - III Floor - Atrium 12:15 - 13:15

Buffet Lunch - Building C11 - Ground Floor - Atrium 13:15 - 14:15

University of Trieste - Department of Chemical and Pharmaceutical Sciences - Building C11 - III Floor - Lecture Hall A3

## MS-11 Interplay between Crystal Growth and Advanced Characterizations for Materials Development

**Chairs: Federico Boscherini** - University of Bologna, **Paola Prete** - Institute for Microelectronics and Microsystems CNR, Lecce

KNL-1 Emanuele Pelucchi - Tyndall National Institute, University College Cork - IE	14:30 - 15:00	MOVPE of III-V Materials: The (Neglected) Role of Surface Dynamics and its Potentials for Next Generation Devices and Integration
KNL-2 Iztok Arčon - University of Nova Gorica - SLO	15:00 - 15:30	Monitoring Chemical Processes in (Photo)Catalysts and Energy Storage Materials by Operando X-Ray Absorption Spectroscopy
O-1 Artur Tuktamyshev - University of Milano "Bicocca", Milano	15:30 - 15:45	Precise structure characterization of droplet epitaxial telecom-wavelength QDs for Quantum Information Technology
O-2 Roberto Bergamaschini - University of Milano "Bicocca", Milano	15:45 - 16:00	Kinetic-control of morphology and composition during the 3D growth of semiconductor nanostructures
O-3 Domenico Mello - STMicroelectronics, Catania	16:00 - 16:15	Defects characterization of GaN heteroepitaxial growth wafer using nSPEC images vs ECCI
O-4 Sandeep Kumar Chaluvadi - Institute of Materials CNR, Trieste	16:15 - 16:30	Direct-ARPES and STM Investigation of FeSe Thin Film Growth by Nd:YAG Laser

Coffee Break - Building C11 - Ground Floor - Atrium 16:30 - 17:00

ePoster Session IV & Commercial Exhibit IV - Building C11 - III Floor - Atrium 17:00 - 18:00

SILS General Assembly - Building C11 - Ground Floor - Main Lecture Hall 18:00 - 20:00

Gala Dinner - Caffè Tommaseo Piazza Nicolò Tommaseo, 4 - Trieste 20:30 - 22:00

# 4<sup>th</sup> Joint AIC-SILS Conference



Trieste September 12-15 2022

Thursday 15<sup>th</sup> September 2022

University of Trieste - Department of Chemical and Pharmaceutical Sciences - Building C11 - Ground Floor - Main Lecture Hall

## Plenary Lecture

PL-4 - Thomas R Schneider - European Molecular Biology Laboratory, Hamburg - DE 08:45 - 09:45 Chair: Michele Cianci - Polytechnic University of Marche, Ancona

Macromolecular crystallography: quo vadis?

Coffee Break - Building C11 - Ground Floor - Atrium

09:45 - 10:15

University of Trieste - Department of Chemical and Pharmaceutical Sciences - Building C11 - III Floor - Lecture Hall A1

## MS-12 Nanostructured Materials

Chair: Paolo Scardi - University of Trento

KNL-1 Jasper Rikkert Plaisier - Elettra-Sincrotrone Trieste, Trieste	10:15 - 10:45	Observing nanomaterials in action using synchrotron radiation
KNL-2 Denis Scaini - Universidad del País Vasco, Vitoria-Gasteiz - ES	10:45 - 11:15	It is just a matter of surfaces: how multidimensional (nano)modifications can modulate neuronal network activity
O-1 Matteo Busato - University of Roma "La Sapienza", Roma	11:15 - 11:30	A multidisciplinary approach to unveil the structural arrangement of deep eutectic solvents: from local order to nano-scale organization
O-2 Gustavo Santiso-Quinones - ELDICO Scientific AG, Villigen - CH	11:30 - 11:45	Structure determination of nanocrystalline MOFs using electron diffraction
O-3 Francesco Tavani - University of Roma "La Sapienza", Roma	11:45 - 12:00	Insights into dissipative and oscillatory chemical reactions by combining X-ray absorption and NMR/UV-Vis spectroscopies
F-1 Alberto Lopez - University of Roma "Roma Tre", Roma	12:00 - 12:05	Exploring anisotropic growth conditions of hydrophilic gold nanorods
F-2 Min Li - University of Bologna	12:05 - 12:10	Crystal structure study of manganese hexacyanoferrate cathode material in organic Na-ion battery by using XAS and XRD
F-3 Alessandro Tofoni - University of Roma "La Sapienza", Roma	12:10 - 12:15	Reversible formation of defects in HKUST-1: a surface perspective by soft X-ray absorption spectroscopy

University of Trieste - Department of Chemical and Pharmaceutical Sciences - Building C11 - Ground Floor - Main Lecture Hall

Best Flash Presentation Prize "Cambridge Crystallographic Data Center"  
Best ePoster Prize "ELDICO Scientific AG"

12:15 - 12:30

Chairs: Chiara Massera - University of Parma, Gustavo Santiso-Quinones - ELDICO Scientific AG, Villigen - CH

Conference Closing Ceremony & Farewell

12:30 - 12:45

Chairs: Francesco Princivalle - University of Trieste, Silvano Geremia - University of Trieste

Angela Altomare - Institute of Crystallography CNR, Bari - President AIC - Conference Chair  
Cinzia Giannini - Institute of Crystallography CNR, Bari - President SILS - Conference Chair  
Federico Boscherini - University of Bologna - Chair of the Conference Scientific Committee  
Doriano Lamba - Institute of Crystallography CNR, Trieste - Chair of the Conference Organizing Committee

Buffet Lunch - Building C11 - Ground Floor - Atrium

12:45 - 13:30

Tour @ Elettra - FERMI

13:30 - 15:30

Upon Request

# 4<sup>th</sup> Joint AIC-SILS Conference



Trieste September 12-15 2022

Thursday 15<sup>th</sup> September 2022

University of Trieste - Department of Chemical and Pharmaceutical Sciences - Building C11 - Ground Floor - Main Lecture Hall

## Plenary Lecture

Chair: **Michele Cianci** - Polytechnic University of Marche, Ancona

PL-4 - **Thomas R Schneider** - European Molecular Biology Laboratory, Hamburg - DE | 08:45 - 09:45 | Macromolecular crystallography: quo vadis?

Coffee Break - Building C11 - Ground Floor - Atrium | 09:45 - 10:15

University of Trieste - Department of Chemical and Pharmaceutical Sciences - Building C11 - III Floor - Lecture Hall A2

## MS-13 Science & Society: from Dissemination to Communication

Chairs: **Paola D'Angelo** - University of Roma "La Sapienza", Roma, **Marta Morana** - University of Pavia

KNL-1 **Chiara Massera** - University of Parma & **Annalisa Guerri** - University of Firenze | 10:15 - 10:45 | Science with and for society: a crystallographic perspective

KNL-2 **Gianluca Santoni** - ESRF, Grenoble - FR | 10:45 - 11:15 | The Coronavirus Structural Task Force

O-1 **Marianna Marchini** - University of Bologna | 11:15 - 11:30 | Grinding in the old times: the synthesis of cinnabar through the glass of ancient recipes

O-2 **Mateja PISAČIĆ** - University of Zagreb - HR | 11:30 - 11:45 | Communicating crystallography through the ECA Lunch webinars

O-3 **Alessia Bacchi** - University of Parma | 11:45 - 12:00 | The power of museums: the case of crystallography in Parma

F-1 **Andrea Ienco** - Institute for the Chemistry of Organometallic Compounds CNR, Sesto Fiorentino | 12:00 - 12:10 | STEM learning paths for high school students

F-2 **Francesco Boni** - Institute of Biophysics CNR, Milano | 12:10 - 12:15 | The CrystalloGame

University of Trieste - Department of Chemical and Pharmaceutical Sciences - Building C11 - Ground Floor - Main Lecture Hall

Best Flash Presentation Prize "Cambridge Crystallographic Data Center"  
Best ePoster Prize "ELDICO Scientific AG"

12:15 - 12:30 | Chairs: **Chiara Massera** - University of Parma, **Gustavo Santiso-Quinones** - ELDICO Scientific AG, Villingen - CH

## Conference Closing Ceremony & Farewell

12:30 - 12:45 | Chairs: **Francesco Princivale** - University of Trieste, **Silvano Geremia** - University of Trieste

**Angela Altomare** - Institute of Crystallography CNR, Bari - **President AIC - Conference Chair**  
**Cinzia Giannini** - Institute of Crystallography CNR, Bari - **President SILS - Conference Chair**  
**Federico Boscherini** - University of Bologna - **Chair of the Conference Scientific Committee**  
**Doriano Lamba** - Institute of Crystallography CNR, Trieste - **Chair of the Conference Organizing Committee**

Buffet Lunch - Building C11 - Ground Floor - Atrium | 12:45 - 13:30

Tour @ Elettra - FERMI | 13:30 - 15:30 | Upon Request

# 4<sup>th</sup> Joint AIC-SILS Conference



Trieste September 12-15 2022

**ePOSTERS Sessions Tuesday 13<sup>th</sup> September 2022 & Wednesday 14<sup>th</sup> September 2022**

**University of Trieste - Department of Chemical and Pharmaceutical Sciences - Building C11 - III Floor - Atrium**

Presenter	Title
<b>MS-01 Modern Integrative Structural Biology</b>	
Flavia Squeglia - Institute of Biostructures and Bioimaging CNR, Napoli	New strategies and tools to fight antimicrobial resistance: A structural point of view
Eliza Kramarska - Institute of Biostructures and Bioimaging CNR, Napoli	The structural approach to vaccine development against ESKAPE pathogens
Andrea Ilari - Institute of Molecular Biology and Pathology CNR, Roma	Structural studies on ornithine decarboxylase from <i>Leishmania infantum</i> , a key enzyme in the polyamine and trypanothione metabolisms
Marta Stefania Semrau - Elettra-Sincrotrone Trieste, Trieste	Molecular architecture of the PTG/PP1 holoenzyme
Stefano Morasso - Elettra-Sincrotrone Trieste, Trieste	A drug repurposing approach targeting SARS-CoV-2 PLpro in the fight against Covid-19
<b>MS-05 Experimental Design &amp; Analysis of Data</b>	
Lucía Mariel Arana Peña - University of Trieste, Trieste	Experimental design for X-Ray phase-contrast microtomography of breast samples for virtual histology
Lorenzo D'Amico - Elettra-Sincrotrone Trieste, Trieste	Towards a multimodal pipeline to characterize lung fibrosis: phase-contrast imaging and porosity analysis
<b>MS-06 Crystallographic and Spectroscopic Advanced Tools Applied to Pharmaceuticals</b>	
Patrizia Rossi - University of Firenze	Investigating the solid form of naproxen-aminoindanol diastereomeric salts
Silvano Geremia - University of Trieste	Specific recognition of methylated lysines by fluorescent calixarenes in protein crystal structures
Mickael Morin - Excelsus Structural Solutions AG, Villingen - CH	Exploring real time amorphization in organic pharmaceutical compounds via in situ ball milling
Theo Battista - University of Trieste	ULK1 inhibition for autophagy deregulation recovery
<b>MS-09 Current Approaches in Structural Biology</b>	
Beatrice De Bonis - University of Siena	Production, characterization, and optimization of engineered enzymes for application in artificial photosynthetic systems
Demi Vattovaz - University of Trieste	Integration of biomolecular simulations and crystallographic approaches to develop enzymes for plastic hydrolysis and recycling
Federico Nolasco - University of Trieste	In silico-designed nanobodies: from the computer to the bench
Thanalai Poonsiri - Free University of Bolzano	Structural and functional characterization of the <i>Aspergillus fumigatus</i> transacylase SidF
<b>MS-10 Investigating Molecular Crystals: Methods and Applications</b>	
Luciano Marchio' - University of Parma	Heptadentate trensal-type ligands for lanthanides coordination and separation
Alma Cioci - University of Torino	The peculiar SHG behavior of solid Co-, Ni- and Cu-porphyrinates
Matteo Melegari - University of Parma	Recovery of rare earth elements from multi-metal mixtures using 8-hydroxyquinolines
Neal Hickey - University of Trieste	X-ray structure investigation of confused-prism[5]arene: a conformationally adaptive host with stereoselective opening of its 1,4-bridged naphthalene flap
Samet Ocak - University of Bologna	Engineering phase change behaviours of organic ionic plastic crystals for development of solid state electrolytes
<b>MS-11 Interplay between Crystal Growth and Advanced Characterizations for Materials Development</b>	
Paola Prete - Institute for Microelectronics and Microsystems CNR, Lecce	MOVPE of GaAsP/GaAs heterostructures for fabrication of 1.7 eV cell junctions in 4-terminal tandem III-V/Si solar cells
Paola Prete - Institute for Microelectronics and Microsystems CNR, Lecce	Graphene nucleation on Si(100): a DFT study on toluene decomposition steps and condensation reactions
Paola Prete - Institute for Microelectronics and Microsystems CNR, Lecce	High efficiency lead-free perovskite solar cells for indoor-outdoor applications
Michele Casappa - University of Parma	Study on pulsed electron deposition as a new method for thin films growth of room temperature multiferroic BaFe <sub>2</sub> O <sub>4</sub>
<b>MS-12 Nanostructured Materials</b>	
Gangadhar Das - Elettra-Sincrotrone Trieste, Trieste	Analysis of TiO <sub>2</sub> nanocomposite using X-ray spectrometry
Lucia Allara - University of Insubria, Como	A deep-learning approach to fast classification of quantum dots size and size dispersion from total scattering data in reciprocal space
Lorenzo Metilli - Université Grenoble Alpes, Grenoble - FR	Self-standing nanoporous zeolite/cellulose deposits prepared with ultrafiltration for energy storage applications