Program

4th Joint AIC - SILS Conference

TRIESTE, 12-15 SEPTEMBER 2022

4th Joint AIC-SILS Conference – Trieste, 12-15 September 2022

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4th Joint AIC-SILS Conference – Trieste, 12-15 September 2022

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Conference Schedule

Monday 12th September 2022

Registration **Parco di San Giovanni - Building N - Meeting Room**	12:00 - 13:45	
Conference Open Cerimony **Parco di San Giovanni - Teatrino Franco Basaglia**	14:00 - 14:30	Chairs:**Francesco Princivalle** - University of Trieste, **Silvano Geremia** - University of Trieste
Roberto Di Lenarda - University of Trieste - **Dean** **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**		
Plenary Lecture		Chair:**Cinzia Giannini** - Institute of Crystallography CNR, Bari -*President SILS*
PL-1 - **Sharon Shwartz** - Bar-Ilan University, Ramat-Gan - ISR	14:30 - 15:30	Quantum imaging with X-rays
Coffee Break	15:30 - 16:00	
Awarding AIC - SILS Prizes		Chairs:**Angela Altomare** - Institute of Crystallography CNR, Bari - *President AIC* , **Cinzia Giannini** - Institute of Crystallography CNR, Bari - *President SILS*
AIC - "Mario Nardelli" Prize *ex- aequo*		
Award Ceremony	16:00 - 16:05	
Paolo Pio Mazzeo - University of Parma	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)
Best PhD Thesis - "Fiorenzo Mazzi" Prizes		
Award Ceremony	16:45 - 16:50	
Rosaria Bruno - University of Calabria	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)
Best BA/MS Thesis - "Fiorenzo Mazzi" Prizes		
Certificate Delivery Ceremony	17:20 - 17:25	
Lisa Baratelli - University of Milano	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 di Milano	17:30 - 17:35	Thermal and compressional behavior of the natural borate kurnakovite, ($MgB_3O_3(OH)_5{\cdot}5H_2O$)
Luca Sironi - University of Milano	17:35 - 17:40	Combined Experimental and Computational Studies on Molecular Recognition among D-Glucose Molecules
SILS - Young Scientist Prize		
Award Ceremony	17:40 - 17:45	
Alberta Terzi - Institute of Crystallography CNR, Bari	17:45 - 18:05	The health seen through collagen network: from disease to regeneration
SILS - PhD Thesis "Carlo Lamberti" Prize		
Award Ceremony	18:05 - 18:10	
Mariele Romano - Ludwig Maximilian University, München - DE	18:10 - 18:20	A multi-technique hierarchical X-ray phase-based approach for the characterization and quantification of the effects of novel radiotherapies
Mineralogy 2022		Chair:**Diego Gatta** - University of Milano - *Past President AIC*
Giuseppe Cruciani - University of Ferrara	18:20 - 18:35	'Mineralogy 2022': a worldwide celebration of mineralogy to highlight its importance in our everyday lives
Panel Discussion ***Horizon-Europe and the Future of Research Infrastructures: Next Generation of Scientific***		Moderator:**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
Questions Time	19:15 - 19:20	
Meeting - AIC Biological MacroMolecules Group *Dip. di Matematica e Geoscienze* **Building O - Lecture Hall A Parco San Giovanni** ***Meeting - AIC Young Crystallographers Group*** *Dip. di Matematica e Geoscienze* **Building O - Lecture Hall B Parco San Giovanni**	19:20 - 20:00	
Welcome Party & Concert of the Ricmanje Orchestra Wind Quintet **Anfiteatro - Roseto Parco di San Giovanni**	20:00 - 21:30	

Tuesday 13th 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 **Marina Mapelli** - European Institute of Oncology, Milano	10:15 - 10:45	Molecular crosstalk between fate determination and orientation in epithelial cell divisions
KNL-2 **Antonio Chaves-Sanjuan** - University of Milano	10:45 - 11:15	Structural characterization of a post-mortem amyloid fibril from a cat kidney
O-1 **Sonia Covaceuszach** - 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 **Benny Danilo Belviso** - 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 **Emiliano De Santis -** University of Uppsala - SE	11:45 - 12:00	Directional explosion. A hybrid simulation study
F-1 **Cecilia Pozzi** - University of Siena	12:00 - 12:05	Structural insights into the hYAP-hTEAD4 protein-protein interaction: an emerging target in cancer treatment
F-2 **Roberto Marotta** - Italian Institute of Technology, Genova	12:05 - 12:10	Unravelling the regulation pathway of photosynthetic AB-GAPDH
F-3 **Francesca Paoletti** - 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 **Andrea Pigozzo** - Alfatest Srl, Roma	12:15 - 12:45	Pushing the boundaries in biomolecular stability and interaction analysis with GCI and MicroCal
S-2 **Max Maletta** - 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 **Paolo Lotti** - University of Milano	14:30 - 15:00	Crystal chemistry of natural REE-phosphates and arsenates and their (T,P)-behavior
KNL-2 **Nicola Campomenosi** - 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 **Mattia La Fortezza** - University of Genova	15:29 - 15:43	Ab initio thermodynamics of $MgSiO_3$ protoenstatite at high temperatures conditions
O-3 **Sabrina Nazzareni** - University of Perugia	15:43 - 15:57	High pressure single-crystal synchrotron XR diffraction of natural pyrochlores
O-2 **Simone Pollastri** - 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 **Sirio Consani** - University of Pisa	16:11 - 16:25	The Cu-Fe-Ni-Co sulphide ore deposits of theMonte Ramazzo-Lagoscuro mines
F-1 **Francesca Menescardi** - 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	

Tuesday 13th 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 **Wilson Crichton** - ESRF, Genoble - FR	10:15 - 10:45	Exploring phase diagrams, structures and properties with the large volume press at the ESRF
KNL-2 **Boby Joseph** - Elettra-Sincrotrone Trieste, Trieste	10:45 - 11:15	Role of crystal lattice in pressure induced electronic transitions : selected examples
O-1 **Marta Morana** - University of Pavia	11:15 - 11:30	X-ray diffraction shines light on mineral inclusions: a natural high-pressure experiment
O-2 **Tommaso Battiston** - University of Milano	11:30 - 11:45	P-mediated crystal-fluid interaction in ERI and OFF topology
O-3 **Benedetta Chrappan Soldavini -** University of Milano	11:45 - 12:00	Structure determination of $CaSiO_3$ wollastonite polymorphs at HP/HT conditions by single crystal in-situ diffraction
F-1 **Maryam Abdolrahimi** - University of Roma "Roma Tre", Roma	12:00 - 12:05	Depth selective local coordination in amorphous $Co_xFe_yB_z$ 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 **Andrea Pigozzo** - Alfatest Srl, Roma	12:15 - 12:45	Pushing the boundaries in biomolecular stability and interaction analysis with GCI and MicroCal
S-2 **Max Maletta** - 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 Milanesio** - University of University of Eastern Piedmont, Alessandria
KNL-1 **Ilaria Carlomagno** - Elettra-Sincrotrone Trieste, Trieste	14:30 - 15:00	Combining experimental and statistical tools for an all-round approach to cultural heritage
KNL-2 **Dmitry Chernyshov** - ESRF, Grenoble - FR	15:00 - 15:30	Synchrotron in situ experimentation, big data, and new tools for fast data processing and analysis
O-1 **Nodoka Hara -** University of Camerino	15:30 - 15:45	Relativistic effects in EXAFS: overview and application to gold
O-2 **Roberta Totani -** 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 **Stevan Vrbaski -** University of Trieste	16:00 - 16:15	Material density and effective atomic number maps of soft tissues via synchrotron radiation spectral CT
F-1 **Mattia Lopresti -** 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 **Gabriele Bonano -** 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	

Tuesday 13th 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 A3

MS-03 Italy@EuXFEL		**Chair:Sakura Pascarelli -** European XFEL, Hamburg - DE
KNL-1 **Matteo Pancaldi** - Elettra-Sincrotrone Trieste, Trieste	10:15 - 10:45	Megahertz-rate ultrafast X-ray scattering and holographic imaging at the European XFEL
KNL-2 **Valerio Cerantola** - European XFEL, Hamburg - DE	10:45 - 11:15	Ultra-fast structural dynamics in materials at extreme conditions
O-1 **Leonardo Martinelli** - Polytechnic University of Milano	11:15 - 11:30	First high energy and temporal resolution pump-probe RIXS at the EuXFEL
O-2 **Valerio Bellucci** - European XFEL, Hamburg - DE	11:30 - 11:45	Fast 4D X-ray imaging at European XFEL
O-3 **Francesco Dallari -** DESY, Hamburg - DE	11:45 - 12:00	Microsecond dynamics in complex liquids with MHz XPCS
O-4 **Oliviero Cannelli** - École Polytechnique Fédérale de Lausanne, Lausanne - CH	12:00 - 12:15	Mapping excitation-specific electron, spin and nuclear dynamics in spinel Co_3O_4 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 **Andrea Pigozzo** - Alfatest Srl, Roma	12:15 - 12:45	Pushing the boundaries in biomolecular stability and interaction analysis with GCI and MicroCal
S-2 **Max Maletta** - 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	

Wednesday 14th 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 Graundery** - 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 α-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 unknow 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 Fermani** - 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	

Wednesday 14th 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_2 electroreduction using time-resolved XAS and advanced data analysis
KNL-2 **Marco Ranocchiari** - 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_2 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	$MZrO_x$ (M = Zn, Ga) catalysts for CO_2 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 unknow 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 Tetrapyridine-Based Crystalline SupramolecularOrganic 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 lenght
O-3 **Mateja Pisačić** - 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	

Wednesday 14th 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 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 Milanesio** - 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 µXRD: 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 biolayer interferometry overview and BLI-MS combination to detect unknow 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	

Thursday 15th 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 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 Scientiifc AG, Villingen - 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***

Thursday 15th 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 Bonì** - 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

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Buffet Lunch - Building C11 - Ground Floor - Atrium	12:45 - 13:30	
Tour @ Elettra - FERMI	13:30 - 15:30	***Upon Request***

ePOSTERs Sessions Tuesday 13th September 2022 & Wednesday 14th September 2022

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

Presenter	Title
MS-01 Modern Integrative Structural Biology	
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 Leishmania infantum, 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
MS-05 Experimental Design & Analysis of Data	
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
MS-06 Crystallographic and Spectroscopic Advanced Tools Applied to Pharmaceuticals	
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
MS-09 Current Approaches in Structural Biology	
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 *Aspergillus fumigatus* transacylase SidF
MS-10 Investigating Molecular Crystals: Methods and Applications	
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
MS-11 Interplay between Crystal Growth and Advanced Characterizations for Materials Development	
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 $BaFe_2O_4$
MS-12 Nanostructured Materials	
Gangadhar Das - Elettra-Sincrotrone Trieste, Trieste	Analysis of TiO_2 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