

4 Joint AIC - SILS Conference

Tuesday 13 September 2022

MS: 1 Modern Integrative Structural Biology - DCPS Building C11/III Floor/- - Lecture Hall A1 (10:15-12:15)

-Conveners: Beatrice Vallone; Stefano Mangani

time	[id] title	presenter
10:15	[1] Molecular Crosstalk between Fate Determination and Orientation in Epithelial Cell Divisions	Dr MAPELLI, Marina
10:45	[2] Structural Characterization of a post-mortem Amyloid Fibril from a Cat Kidney	Dr CHAVES SANJUAN, Antonio
11:15	[74] Insights on the structural determinants of proBDNF V66M variant, a modifier in neuropsychiatric disorders severity.	Dr COVACEUSZACH, Sonia
11:30	[94] C-terminus of the histone-lysine N-methyltransferase NSD3 characterized by small-angle X-ray scattering	Dr BELVISO, Benny Danilo
11:45	[125] Directional explosion. A hybrid simulation study	DE SANTIS, Emiliano
12:00	[105] Structural insights into the hYAP-hTEAD4 protein-protein interaction: an emerging target in cancer treatment	Prof. POZZI, Cecilia
12:05	[115] Unravelling the regulation pathway of photosynthetic AB-GAPDH	MAROTTA, Roberto
12:10	[96] Landscape of the ATP binding to neurotrophins: effects on conformation and dynamic modulation by divalent cations	Dr PAOLETTI, Francesca

MS: 7 Materials at Extreme Conditions: X-ray Crystallography and Beyond - DCPS Building C11/III Floor/- - Lecture Hall A2 (10:15-12:15)

-Conveners: Davide Comboni; Giuliana Aquilanti

time	[id] title	presenter
10:15	[13] Exploring Phase Diagrams, Structures and Properties with the Large Volume Press at the ESRF	Dr CRICHTON, Wilson
10:45	[14] Role of crystal lattice in pressure induced electronic transitions: selected examples	Dr JOSEPH, Boby
11:15	[30] X-ray diffraction shines light on mineral inclusions: A natural high-pressure experiment	MORANA, Marta
11:30	[33] P-mediated crystal-fluid interaction in ERI and OFF topology	Mr BATTISTON, Tommaso
11:45	[79] Structure determination of CaSiO ₃ wollastonite polymorphs at HP/HT conditions by single crystal in-situ diffraction	CHRAPPAN SOLDAVINI, Benedetta
12:00	[90] Depth selective local coordination in amorphous CoxFeyBz thin films probed by XAFS under x-ray standing wave condition	ABDOLRAHIMI, Maryam

MS: 3 Italy@EuXFEL - DCPS Building C11/III Floor/- - Lecture Hall A3 (10:15-12:15)

-Conveners: Sakura Pascarelli

time	[id] title	presenter
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10:15	[69] Megahertz-rate Ultrafast X-ray Scattering and Holographic Imaging at the European XFEL	Dr PANCALDI, Matteo
10:45	[6] Ultra-fast structural dynamics in materials at extreme conditions	Dr CERANTOLA, Valerio
11:15	[81] First high energy and temporal resolution pump-probe RIXS at the EuXFEL	MARTINELLI, Leonardo
11:30	[153] Fast 4D X-ray Imaging at European XFEL	BELLUCCI, Valerio
11:45	[97] Microsecond dynamics in complex liquids with MHz XPCS	Dr DALLARI, Francesco
12:00	[130] Mapping excitation-specific electron, spin and nuclear dynamics in spinel Co ₃ O ₄ thin films with femtosecond X-ray emission spectroscopy and diffraction	Dr CANNELLI, Oliviero

MS: 5 Experimental Design & Analysis of Data - DCPS Building C11/III Floor/- - Lecture Hall A2 (14:30-16:30)

-Conveners: Marco Milanesio

time	[id] title	presenter
14:30	[9] Combining Experimental and Statistical Tools for an All-round Approach to Cultural Heritage	Dr CARLOMAGNO, Ilaria
15:00	[10] Synchrotron in situ Experimentation, Big data, and New Tools for Fast Data Processing and Analysis	Dr CHERNYSHOV, Dmitry
15:30	[155] Relativistic effects in EXAFS: overview and application to gold	HARA, Nodoka
15:45	[109] Spectroscopic investigations of nitroxide persistent organic radicals. Future perspectives in view of Elettra 2.0: the MOST beamline	Dr TOTANI, Roberta
16:00	[119] Material density and effective atomic number maps of soft tissues via synchrotron radiation spectral CT	VRBASKI, Stevan
16:15	[61] Principal component scores projection on a barycentric coordinate system for a quantification in polycrystalline mixtures XRPD data without crystal structure data	Dr LOPRESTI, Mattia
16:20	[128] Thin liquid flat-jet for spectroscopy in the soft x-ray photon energy range	BONANO, Gabriele

MS: 4 Frontiers in Mineralogy and Inorganic Geochemistry - DCPS Building C11/III Floor/- - Lecture Hall A1 (14:30-16:30)

-Conveners: Donato Belmonte; Gabriele Giuli

time	[id] title	presenter
14:30	[7] Crystal Chemistry of Natural REE-Phosphates and Arsenates and their (T,P)-Behavior	Dr LOTTI, Paolo
15:00	[8] Elastic vs. Visco-plastic Rheology of Stressed Host-Inclusion Mineral Systems at non-Ambient Conditions: Insights from in situ Raman Spectroscopy	Dr CAMPOMENOSI, Nicola
15:29	[32] Ab initio thermodynamics of MgSiO ₃ protoenstatite at high temperatures conditions	Dr LA FORTEZZA, Mattia
15:43	[102] High Pressure Single-crystal Synchrotron XR diffraction of natural pyrochlores	Dr NAZZARENI, Sabrina
15:57	[42] Characterization of bottom ashes from incineration process by means of XRF mapping and XANES spectroscopy	POLLASTRI, Simone
16:11	[122] The Cu-Fe-Ni-Co Sulphide Ore Deposits of the Monte Ramazzo-Lagoscuoro Mines	Dr CONSANI, Sirio
16:25	[29] Molecular dynamics strategies to determine the melting curve of CaO	Dr MENESCARDI, Francesca

Wednesday 14 September 2022

MS: 8 Bright Radiation Sources and Novel Software Applications - DCPS Building C11/III Floor/- - Lecture Hall A3 (10:15-12:15)

-Conveners: Corrado Cuocci; Francesco Stellato

time	[id] title	presenter
10:15	[15] Solid State NMR Spectroscopy with Quantum Espresso	Dr CERESOLI, Davide
10:45	[16] Ultrafast X-ray Sources: an Opportunity for Science	Dr PRINCIPI, Emiliano
11:15	[43] The EuPRAXIA FEL project: ultra-bright light pulses for imaging and spectroscopy	Dr EBRAHIMPOUR, Zeinab
11:30	[107] A machine learning-based web platform for crystal system classification: CrystalMELA	Dr CORRIERO, NICOLA
11:45	[108] PCA analysis of in situ X-ray powder diffraction and imaging data: new approaches named differential scanning diffraction and imaging	MILANESIO, Marco
12:00	[82] Unattended MX data collection and beamline monitoring at Diamond	Dr MAZZORANA, Marco
12:05	[88] XRD2 to μ XRD: Italian Beamlines Dedicated to Macromolecular Crystallography	HEROUX, Annie

MS: 2 Understanding Advanced Functional Materials Through Operando Studies - DCPS Building C11/III Floor/- - Lecture Hall A2 (10:15-12:15)

-Conveners: Elisa Borfecchia; Simona Galli

time	[id] title	presenter
10:15	[3] Understanding the Structure-Properties Relationship in Nanocatalysts for CO ₂ Electroreduction using Time-Resolved XAS and Advanced Data Analysis	Dr TIMOSHENKO, Janis
10:45	[4] Characterization of Metal-Organic Frameworks with Synchrotron and Neutron Sources for Catalytic Applications	Dr RANOCCHIARI, Marco
11:15	[39] Operando and ex-situ PXRD Study of Ni-doped Manganese Hexacyanoferrate Cathode Material in Aqueous Zn-ion Battery System	MAISURADZE, Mariam
11:30	[152] Tracking the evolution of Ni-based single atom catalysts for the CO ₂ electroreduction reaction: an operando XAS study assisted by machine learning techniques	MARTINI, Andrea
11:45	[138] On the mechanism of cocrystal mechanochemical reaction via low melting eutectic: a time resolved in-situ monitoring investigation	MAZZEO, Paolo P.
12:00	[50] MZrO _x (M = Zn, Ga) catalysts for CO ₂ hydrogenation reaction: exploiting XAS and PXRD to understand catalyst's structure, activity and stability	SALUSSO, Davide
12:05	[65] Hg(II)-Bispidine 1D Coordination Polymers: three different topologies and their dynamic behavior in solvent adsorption and exchange processes	Dr LIPPI, Martina

MS: 6 Crystallographic and Spectroscopic Advanced Tools Applied to Pharmaceuticals - DCPS Building C11/III Floor/- - Lecture Hall A1 (10:15-12:15)

-Conveners: Fabia Gozzo

time	[id] title	presenter
10:15	[11] Structural Insights into TRPM Channels. A Long and Unexpected Journey	Dr TALARICO, Carmine

10:45	[12] Relevance of solid form's curriculum for drug product development: beyond polymorphism of drug substance	Dr GRANDEURY, Arnaud
11:15	[104] The "Form Selection Process" in the Pharmaceutical Industry: the importance of being Earnest	Dr DALDOSSO, Matteo
11:30	[154] Advances in the quantification of amorphous pharmaceuticals via Multivariate Analysis of Synchrotron X-Ray Powder Diffraction Patterns	REINLE-SCHMITT, Mathilde
11:45	[114] The structural biology task force at Elettra to support drug discovery against Covid-19	STORICI, Paola
12:00	[57] Structural characterization of human Heat shock protein 90 N-terminal domain in complex with a potent 1,2,3-triazole based inhibitor	Dr TASSONE, Giusy
12:05	[100] Prediction of hERG-Mediated Cardiotoxicity based on the integration of docking scores and protein–ligand interaction fingerprints	Dr DELRE, Pietro
12:10	[127] Unusual binding ability of anticoagulant aptamers revealed by the crystallographic analysis of an engineered pseudo-cyclic TBA in complex with α -thrombin	TROISI, Romualdo

MS: 9 Current Approaches in Structural Biology - DCPS Building C11/III Floor/- - Lecture Hall A1 (14:30-16:30)

-Conveners: Michele Cianci; Simona Fermani

time	[id] title	presenter
14:30	[17] X-Ray Crystallography for Vaccine Development Against Emerging Pathogens	Dr BERISIO, Rita
15:00	[18] 3D Electron Diffraction of Beam Sensitive Samples of Biological Interest: Proteins and Pharmaceuticals	Dr GEMMI, Mauro
15:30	[68] Single particle cryo-EM unveils multiple states in PdxR mechanism of transcriptional regulation	FREDA, Ida
15:45	[135] Towards the Cryo-EM structure of the ERAD glycoprotein folding checkpoint, the EDEM:PDI heterodimer.	HITCHMAN, Charles J
16:00	[95] RNA-viruses inhibitors: unintended consequences of the target driven approach	MASTRANGELO, ELOISE
16:15	[48] Fully autonomous end-to-end protein to structure pipelines at MASSIF-1 using the CrystalDirect harvester	ROCCHIO, Serena
16:20	[54] Characterization of Ca-depositions evolution by cryo-XANES and cryo-STX in SaOS-2 osteosarcoma cells	ROSSI, Francesca
16:25	[84] Glycation in collagen macromolecule of diabetic biotissues	TERZI, Alberta

MS: 10 Investigating Molecular Crystals: Methods and Applications - DCPS Building C11/III Floor/- - Lecture Hall A2 (14:30-16:30)

-Conveners: Alessandra Forni; Emanuele Priola

time	[id] title	presenter
14:30	[19] Refining Structures of Molecular Crystals through Modern Methods of Quantum Crystallography	Prof. GENONI, Alessandro
15:00	[20] From Crystallography to Physical Properties: What the Second Harmonic Generation Property Is Due To?	Dr MARABELLO, Domenica
15:30	[35] Dynamic Behaviour of a Tetrapyrroline-Based Crystalline SupramolecularOrganic Framework	MARCHETTI, Danilo

15:45	[113] Porous and luminescent coordination complexes and networks assembled from a new ligand of nanometric length	CARLUCCI, Lucia
16:00	[66] Shaping crystals using mechanical force: A structural perspective on flexible crystalline coordination polymers of cadmium(II)	Ms PISAČIĆ, Mateja
16:15	[55] Exploring weak interactions realm with cyclic peptoids	Dr PIERRI, Giovanni
16:20	[63] Cocrystallization as effective tool for driving the release of natural active compounds	PRENCIPE, Michele
16:25	[71] Crystal Engineering as a tool for rational design of novel sustainable food, agrochemical and pharmaceutical formulations	SIMONE, Elena

MS: 11 Interplay between Crystal Growth and Advanced Characterizations for Materials Development - DCPS Building C11/III Floor/- - Lecture Hall A3 (14:30-16:30)

-Conveners: Federico Boscherini; Paola Prete

time	[id] title	presenter
14:30	[22] MOVPE of III-V Materials: The (Neglected) Role of Surface Dynamics and its Potentials for Next Generation Devices and Integration	Dr PELUCCHI, Emanuele
15:00	[21] Monitoring Chemical Processes in (Photo)Catalysts and Energy Storage Materials by Operando X-Ray Absorption Spectroscopy	Prof. IZTOK, Arčon
15:30	[83] Precise structure characterization of droplet epitaxial telecom-wavelength QDs for Quantum Information Technology	Dr TUKTAMYSHEV, Artur
15:45	[137] Kinetic-control of morphology and composition during the 3D growth of semiconductor nanostructures	Dr BERGAMASCHINI, Roberto
16:00	[80] Defects characterization of GaN heteroepitaxial growth wafer using nSPEC images vs ECCI	MELLO, Domenico
16:15	[151] Direct-ARPES and STM Investigation of FeSe Thin Film Growth by Nd:YAG Laser	Dr CHALUVADI, Sandeep Kumar

Thursday 15 September 2022

MS: 12 Nanostructured Materials - DCPS Building C11/III Floor/- - Lecture Hall A1 (10:15-12:15)

-Conveners: Paolo Scardi

time	[id] title	presenter
10:15	[23] Observing Nanomaterials in Action Using Synchrotron Radiation	Dr PLAISIER, Jasper
10:45	[24] It is just a matter of surfaces: how multidimensional (nano)modifications can modulate neuronal network activity	Prof. SCAINI, Denis
11:15	[64] A Multidisciplinary Approach to Unveil the Structural Arrangement of Deep Eutectic Solvents: from Local Order to Nano-scale Organization	Dr BUSATO, Matteo
11:30	[76] Structure Determination of Nanocrystalline MOFs Using Electron Diffraction	Dr SANTISO-QUINONES, Gustavo
11:45	[78] Insights into dissipative and oscillatory chemical reactions by combining X-ray absorption and NMR/UV-Vis spectroscopies	TAVANI, Francesco
12:00	[91] Exploring anisotropic growth conditions of hydrophilic gold nanorods.	Dr LOPEZ, Alberto Dr VENDITTI, Iole
12:05	[37] Crystal Structure Study of Manganese Hexacyanoferrate Cathode Material in Organic Na-ion Battery by using XAS and XRD	Ms LI, Min
12:10	[70] Reversible formation of defects in HKUST-1: a surface perspective by Soft X-ray Absorption Spectroscopy	Mr TOFONI, Alessandro

MS: 13 Science & Society: from Dissemination to Communication - DCPS Building C11/III Floor/- - Lecture Hall A2 (10:15-12:15)

-Conveners: Marta Morana; Paola D'Angelo

time	[id] title	presenter
10:15	[25] The Coronavirus Structural Taskforce	Dr SANTONI, Gianluca
10:45	[26] Science with and for Society: A Crystallographic Perspective	Dr GUERRI, Annalisa Prof. MASSERA, Chiara
11:15	[93] Grinding in the old times: the synthesis of cinnabar through the glass of ancient recipes	MARCHINI, Marianna
11:30	[67] Communicating crystallography through the ECA Lunch webinars	Ms PISAČIĆ, Mateja
11:45	[56] The Power of Museums: the case of Crystallography in Parma	Prof. BACCHI, Alessia
12:00	[131] STEM Learning Paths for High School Students	Dr IENCO, Andrea
12:10	[77] The Crystallogame	BONI, Francesco