

# Meeting Program

**Monday, September 15 2014**

Aula Magna Rettorato, Università degli Studi di Firenze, P.zza S. Marco 4

12:00-14:00: Registration

14:00 – 14:30: **Open Ceremony:** Welcome from authorities

(Chairs: Michele Saviano, AIC President, Federico Boscherini, SILS President)

14:00 – 14:10: Prof. **Alberto Tesi**, dean of the University of Florence

14:10 - 14:20: Prof. **Cristina Giachi**, deputy mayor of the city of Florence

14:20 – 14:30: Dr. **Luigi Ambrosio**, Director of the Chemical Sciences and Materials Technology Department, CNR.

14:30 – 15:15: **Plenary Lectures** (Chair: Carlo Mealli)

**Marine Cotte** “Synchrotron-based Micro-analytical Techniques in the Studies of Art and Historical Artifacts”

15:15 – 15:40: **AICNardelli Prize** (Chair: Michele Saviano)

**Rossella Arletti** “Impose Pressure and Change Technology: Pressure-induced intrusion and organized nanostructures in zeolites”

15:40 – 15:55: **AIC Ph.D. Thesis Award** (Chair: Michele Saviano)

**Paolo Lotti** "Cancrinite-group minerals at non-ambient conditions: a model of the elastic behavior and structure evolution"

15:55 – 16:00: **AIC Master Degree Thesis Award** (Chair: Michele Saviano)

**Valentina Loconte**(Poster #1)

16:00-16:20: **SILS-BioGem Award for bio-medical applications** (Chair: Federico Boscherini)

**Enrico Junior Baldassarri** “Unravelling the Counter-ion Effects on

Guanosine Self-Assembly: an Extended Structural Study”

16:20-16:40: **SILS–SPECS Award** (Chair: Federico Boscherini)

**Mattea Carmen Castrovilli** “Elementary processes of radiation damage  
in organic molecules of biological interest”

16:40-17:00: **SILS-BRUKER Ph.D. Award** (Chair: Federico Boscherini)

**Lara Gigli** “Synchrotron XRPD evidence of highly organized dye  
molecules in 1D nanochannels of Zeolite L”

17:00-17:30: **Coffee break**

17:30-17:45: **Celebration of the International Year of Crystallography** (Chair:  
Alessia Bacchi)

17:45-18:15: **Daide Viterbo** “Incontri ravvicinati con cristallografi che ne hanno  
fatto la storia”

18:15-18:45: **Luigi Dei** “Cristalli, musica, poesia: è tutta questione di simmetria!”

## **Tuesday, September 16 2014**

Chiostro del Maglio, via Venezia, 5

9:00–9:45: **Plenary Lecture** (Chair: Giuseppe Zanotti)

**Dmitri Svergun** “Synergistic use of Biological Small Angle X-ray Scattering with Macromolecular Crystallography”

9:45-10:15: **Coffee Break**

### **10:15-12:15: MS1 & MS6**

#### **MS1:Structural Biology at High and Low Angles**

Chairs: Paolo Mariani, Massimiliano Perduca (Auditorium)

10:15-10:45: **Silvia Onesti** “Macromolecular machines involved in DNA replication: an integrated structural biology approach”

10:45- 11:15: **Adam Round** “BioSAXS – Current possibilities for low resolution structural and functional studies”

11:15-11:35: **Daniele de Sanctis** “The ESRF Structural Biology beamlines”

11:35-11:55: **Michele Cianci** “EMBL P13 beamline at PETRA III @DESY: harnessing sulfur anomalous signal from biological macromolecules with a 4.6keV X-ray beam”

11:55-12:15: **Alessandra Del Giudice** “Structural insights into the shape and assembly of photosynthetic GAPDH/CP12/PRK complex by small angle X-ray scattering”

#### **MS6:Nano-Crystal Growth and Characterization**

Chairs: Massimo Longo, Silvia Milita (Conference Room)

10:15-10:45: **Lucia Sorba** “Growth of III-V nanowires: from fundamental physics to device applications”

10:45- 11:15: **Giuseppe Nicotra** “Advanced characterisation from the nanoscale to the single atom through (S)TEM”

11:15-11:35: **Davide Calestani** “Surface functionalization of ZnO nanostructures: designing material properties at nanoscale”

11:35-11:55: **Antonella Guagliardi** “Unravelling the Growth of Pt Nanorods inside a Porous Matrix by Total Scattering Debye Function Analysis”

11:55-12:15: **Giulio Isacco Lampronti** “Direct observation of intermediates in a thermodynamically controlled solid-state dynamic covalent reaction”

### **12:15-13:15: Commercial Presentation I (Auditorium)**

12:15-12:35: **Lucia Robba** (Bruker) “True data of the real nanoworld – N8 HORIZON”

12:35-12:55: **Dubravka Šišak Jung** (Dectris) “Advanced X-ray diffraction analysis using single-photon-counting detectors”

12:55-13:15: **Paul Pennartz** (Rigaku): “New 2D detectors and solutions for Rigaku SmartLab(tm) Systems and recent developments in X-ray optics”

### **13:15-14:30 Lunch & Poster Session**

## **14:30-16:30: MS3 & MS4**

### **MS3: Probing Structure, Properties and Transformation Processes of Materials under Extreme Conditions**

Chairs: Marco Merlini, Nicola Casati (Auditorium)

14:30-15:00: **Mario Santoro** “High pressure synthesis of novel materials”

15:00-15:30: **Michael Hanfland** “Crystallography at extreme conditions”

15:30-15:50: **Ross John Angel** “EosFit7: A new program for equation of state analysis”

15:50-16:10: **Raffaella Torchio** “High pressure and low temperature structure and magnetism of cobalt”

16:10-16:30: **Arianna Lanza** “Pressure-induced structural and magnetic transformations in  $[(\text{CuF}_2(\text{H}_2\text{O})_2)_x(\text{pyz})]$  polymers”

#### **MS4: New Frontiers in Methods and Techniques**

Chairs: Ralf Menk, Dritan Siliqi (Conference Room)

14:30-15:00: **Cinzia Giannini** “Exploiting high brilliance synchrotron-like micro-focused beams in a table-top facility to study nano- and bio-materials”

15:00-15:30: **Bernd Schmitt** “Beyond PILATUS and Mythen: New frontier detectors for x-ray diffraction”

15:30-15:50: **Francesco Carlà** “In-situ Investigation of Electrochemical Growth Processes by Surface X-ray Diffraction”

15:50-16:10: **Piero Torelli** “APE beamline: a spectroscopic tool toward the investigation of magnetic properties in-operando conditions”

16:10-16:30: **Nicola Corriero** “QUALX2.0: a qualitative analysis program inquiring a freely available database”

16:30-16:50 **Coffee Break**

**16:50-18:35: Large Scale Facilities Updates** (Chair: Federico Boscherini)

(Auditorium)

16:50-17:15: **Francesco Sette**: ESRF

17:15-17:40: **Maya Kiskinova** Elettra and FERMI

17:40-17:55: **Gianluca Geloni**: XFEL

17:55-18:10: **Giorgio Rossi**: ESFRI (European Strategy Forum on Research Infrastructures)

18:10-18:25: **Giacomo Ghirighelli**: CNR Commission of Synchrotron Radiation

and Neutrons

18:25-18:35: **Massimo Ferrario**: Activities in Frascati

18:40-19:30: **SILS Assembly** (Auditorium)

20:30: Social Dinner at **Palazzo Borghese**

**Wednesday, September 17 2014**

Chiostro del Maglio, via Venezia, 5

9:00–9:45: **Plenary Lecture** (Chair: Diego Gatta)

**Christian Serre** “From in/ex situ studies to applications of porous MOFs”

9:45-10:15: **Coffee Break**

**10:15-12:15: MS5 & MS2**

**MS5:News from the Crystal-Chemistry of Inorganic Compounds: from Nature to Tailor-Made Materials**

Chairs: Giuseppe Cruciani , Ferdinando Costantino (Auditorium)

10:15-10:45: **Angiolina Comotti** “In situ polymerization and rotor dynamics in Porous Materials”

10:45-11:15: **Enrico Mugnaioli** “Biominerals by electron and synchrotron X-ray powder diffraction”

11:15-11:35: **Maria Victoria-Rodríguez** “Gas adsorption study on HKUST-1 of different particle size”

11:35-11:55: **Elisa Boanini** “Interaction of Calcium Phosphates with Bisphosphonates: from Composite Crystals to Calcium Phosphates Digestion”

11:55-12:15: **Matteo Ardit** “Spontaneous strain variation and thermodynamic properties through the monoclinic/ orthorhombic phase transition of ZSM-5 zeolite”

## **MS2: Industrial Applications of Crystallography and Synchrotron Radiation**

Chairs: Marco Peloi, FabiaGozzo (Conference Room)

10:15-10:45: **Bernd Hinrichsen** “Shedding light on the Structure of Novel Perovskite Photovoltaic Material”

10:45-11:15: **Roberto Millini** “Crystallography in an Industrial Research Laboratory: the experience of ENI”

11:15-11:35: **Nicola Casati** “Time is money: high throughput synchrotron XRPD”

11:35-11:55: **Ed Mitchel** “Industry at synchrotrons: a necessary evil or a win-win situation?”

11:55-12:15: **Lucia Maini** “Multivariate analysis and Rietveld refinement for quantification of inorganic additives in animal feeds”

### **12:15-12:55: Commercial Presentation II (Auditorium)**

12:15-12:35: **ZoltánGál** (Agilent): “Use of a single crystal diffractometer for polycrystalline sample characterization”

12:35-12:55: **Eric Hovestreydt** (Bruker): “Light-Atom Absolute Configuration Determination at Different Wavelengths”

### **12:55-14:30 Lunch & Poster Session**

## **14:30-16:30: MS7 & MS8**

### **MS7:Nano and Advanced Materials: the Diffraction and Spectroscopy Points of View**

Chairs: Alberto Morgante, Matteo Leoni (Auditorium)

14:30: 15:00: **Elisa Miniussi** “Fine Tuning of Graphene-Metal Interaction”

15:00-15:30: **Luca Palin** “Investigation of layered and disordered materials by XRPD Raman and NMR”

15:30-15:50: **AntonellaIadecola** “Local structure of nanostructured V<sub>2</sub>O<sub>5</sub> probed by x-ray absorption spectroscopy”



15:50-16:10: **Paolo Moras** “Free-standing vs. Ag(111)-supported: substrate effects on silicene properties”

16:10-16:30: **Lise Pascale** “Evidence of superconductivity in ordered tetragonal  $\text{YBa}_2\text{Cu}_3\text{O}_{7-x}$  micro-crystals induced by chemical substitution”

### **MS8:Advanced Radiation Sources**

Chairs: Enrica Chiadroni, Andrea Lausi (Conference Room)

14:30: 15:00: **Leonida Antonio Gizzi** “All-optical X-ray and gamma-ray sources driven by ultraintense lasers”

15:00-15:30: **Riccardo Cucini** “Time resolved nanoscale dynamics in condensed matter: The TIMER project”

15:30-15:50: **Stefano Lupi** “Terahertz Radiation for Non linear and Pump-Probe Spectroscopy”

15:50-16:10: **Fabio Villa** “Two colors FEL at SPARC\_LAB”

16:10-16:30: **Alberto Bacci** “Physics and Perspectives of Thomson/Compton Sources”

16:30-17:00: **Coffee Break**

### **End of the Joint SILS – AIC Congress**

17:00-19:00: **AIC General Assembly**(Auditorium)

**Thursday, September 18 2014**

Chiostro del Maglio, via Venezia, 5

9:00–9:45: **Plenary Lecture** (Chair: Patrizia Rossi)

**Davide M. Proserpio** “Periodic Structures and Crystal Chemistry: A history of the topological approach to crystal chemistry by means of the cds net”.

9:45-10:15: **Coffee Break**

**10:15-12:35: MS9 & MS10**

**MS9:Structure-Property Correlation in Molecular Crystals**

**Chair:** Roberto Centore (Auditorium)

10:15-10:45: **Alessandra Crispini** “Intermolecular interactions in the design of molecular materials and their properties”

10:45-11:15: **Fabrizia Grepioni** “From drugs to pigments and sensors: cocrystallization as a flexible tool for properties enhancement of molecular materials”

11:15-11:35: **Davide Capucci** “Trapping liquid drugs in cocrystals and MOFs”

11:35-11:55: **Fabiola Liscio** “Does the organic field effect transistor operation affect molecular film structure?”

11:55-12:15: **Werner Oberhauser** “Linear  $\alpha$ -Olefins Obtained with Structural Isomers of a Dinuclear Palladium Tetra-phosphanedioxide Complex”

12:15-12:35: **Consiglia Tedesco** “Towards the control of the solid state assembly of cyclic peptoids”

## **MS10:Mathematical Crystallography**

**Chair:** Stefano Leoni (Conference Room)

10:15-10:45: **Charlotte Bonneau** “Why do we have to learn about crystal nets?”

10:45-11:15: **ArinaPankowa** “New Tools for Taxonomy of Nanoclusters in Intermetallics”

11:15-11:35: **Mario Valle** “Crystal fingerprints space a novel paradigm to study crystal structures sets”

11:35-11:55: **Igor Baburin** “From abstract nets to chemical compounds: applications to porous solids”

11:55-12:15: **SenjaBarthel** “How knot theory can contribute to crystallography (tangled and braided structures)”

12:15-12:35: **RuggeroGabbrielli** “Periodic simple tiling as models for monodispersed foam”

12:35-13:00: **AIC ClosingCeremony** (Auditorium)