

**MEETING OF THE ITALIAN, SPANISH AND SWISS  
CRYSTALLOGRAPHIC ASSOCIATIONS**

**SEPTEMBER, 9<sup>th</sup> – 12<sup>th</sup> 2013, VILLA OLMO, COMO (ITALY)**

**SCIENTIFIC PROGRAM**

**Monday, September 9<sup>th</sup>, 2013**

- 13:00-15:00 Registration
- 15:00-15:30 Opening Ceremony
- 15:30-16:30 **PL1: Stuart S.P. PARKIN**, IBM San José, USA  
*Turning insulators into metals!*  
Chair: **Jürg SCHEFER**
- 16:30-18:00 **PRIZES**  
Chairs: **Michele SAVIANO** and **Fernando LAHOZ**
- 16:35-17:05 **AIC Nardelli Prize 2013**  
**Laura CENDRON**, Università di Padova, Italy  
*Structural and functional studies on HydF, an enzyme with a key role in the maturation of the [FeFe]-hydrogenase catalytic core*
- 17:05-17:35 **AIC Prize for the best PhD thesis**  
**Mauro CODURI**, Università di Milano, Italy  
*Local disorder in doped ceria: from low temperature to operating conditions*  
**Eleonora CONTEROSITO**, Università del Piemonte Orientale, Italy  
*Optimization of intercalation yield into hydrotalcites by liquid assisted grinding*
- 17:35-17:45 **AIC Prize for the best graduation thesis**  
**Elisa BONNINI**, IMEM-CNR Institute, Italy  
*Curved focussing crystals for hard X-ray astronomy*  
**Giorgia CONFALONIERI**, Università di Milano, Italy  
*Local distortions in the structure of nanocrystalline gahnite*

- 17:45-18:00            **GE3C Xavier Solans Prize 2013**  
Introduction by: **Fernando LAHOZ**
- 18:00-18:30            **AIC Mammi Prize 2013**  
**Roberta OBERTI**, CNR-Istituto di Geoscienze e Georisorse, UOS  
Pavia, Italy  
*Chipping, baking and squeezing amphiboles (and more):  
the importance of crystal-chemical models*
- 18:30-19.00            **MISCA Medal 2013**  
**Juan Manuel GARCÍA-RUIZ**, Laboratorio de Estudios  
Cristalográficos, IACT-CSIC-UGR, Spain  
*Crystals and (my) life*
- 20:00-22:00            **Welcome Party at Villa Olmo**

## **Tuesday, September 10<sup>th</sup>, 2013**

- 9:00-10:00            **PL2: Tilman SCHIRMER**, University of Basel,  
Switzerland  
*Mechanisms to regulate the cellular concentration  
of the bacterial second messenger c-di-GMP*  
Chair: **Michele SAVIANO**
- 10:00-10:30           **Coffee Break**
- 10:30-12:00           **MS1: MACROMOLECULAR ASSEMBLIES AND VIRUSES**  
Chair: **María SOLÀ**
- (Oval Room)*
- 10:30-11:00           **KN1: Guillermo MONTROYA**, Centro Nacional de  
Investigaciones Oncológicas, Spain  
*Macromolecular complexes and hybrid methods a well  
set marriage: an example from the TRiC/tubulin  
crystal structure*
- 11:00-11:20           **O1.1: Antonio CHAVES SANJUÁN**, Instituto de Química-  
Física “Rocasolano”, CSIC, Spain  
*The structure of the CBL-CIPK pathway: the  
regulation of Arabidopsis thaliana ion homeostasis*
- 11:20-11:40           **O1.2: Gianpiero GARAU**, Istituto Italiano di  
Tecnologia, Italy  
*Biogenesis of endogenous lipid amide signals*
- 11:40-12:00           **O1.3: Andrea ILARI**, Istituto di Biologia e Patologia  
Molecolari, CNR, Italy  
*The X-ray structures of tryparedoxin and tryparedoxin  
peroxidase reveal the molecular mechanism of  
peroxide reduction in Leishmania parasites*
- 10:30-12:00           **MS2: STRUCTURE AND PROPERTIES OF INORGANIC  
AND ORGANIC THIN FILMS**  
Chair: **Adele SASSELLA**
- (Ball Room)*
- 10:30-11:00           **KN2: Frank SCHREIBER**, Universität Tübingen, Germany  
*Real-time X-ray scattering studies of thin film growth*

- 11:00-11:20 O2.1: **Evelyn MORENO-CALVO**, Institut de Ciència de Materials de Barcelona, Spain  
*Quatsomes: vesicular structures formed by self-assembly of sterols and quaternary ammonium surfactants*
- 11:20-11:40 O2.2: **Paolo P. MAZZEO**, Università di Bologna, Italy  
*New copper(I) complexes: structures and photochemical characterization in solid state for OLEDs devices*
- 11:40-12:00 O2.3: **Fabiola LISCIO**, Istituto per la Microelettronica e Microsistemi, Italy  
*Control of octathiophene fibers orientation fabricated by lithographically wetting process*
- 12:00-12:30 **COMMERCIAL PRESENTATIONS #1**  
*(Ball Room)*
- 12:00-12:15 C1.1: **Martin ADAM**, Bruker AXS, Germany  
*100 days of PHOTON 100 CMOS detector Experience*
- 12:15-12:30 C1.2: **Jürgen GRAF**, Incoatec GmbH, Germany  
*Beam conditioning in cutting edge X-ray analytical equipment*
- 12:30-14:00 **Lunch**
- 14:00-15:00 **POSTER SESSION P1: MS1, MS2, MS3, MS5, MS6**
- 15:00-16:30 **MS3: FRONTIERS IN INSTRUMENTATION**  
Chair: **Vladimir DMITRIEV**  
*(Oval Room)*
- 15:00-15:30 KN3: **Ian K. ROBINSON**, London Centre for Nanotechnology, UCL, United Kingdom  
*Opportunities for coherence in crystallography*
- 15:30-15:50 O3.1: **Jürg SCHEFER**, Paul Scherrer Institut, Villigen, Switzerland  
*HEIMDAL: a time-of-flight neutron powder diffractometer going beyond today's designs by offering additionally a SANS and an imaging option*

- 15:50-16:10 O3.2: **Vadim DYADKIN**, Swiss-Norwegian Beamline at the European Synchrotron Radiation Facility, France  
*Pilatus@SNBL: new multi-purpose diffractometer based on Pilatus 2M pixel area detector*
- 16:10-16:30 O3.3: **Jasper PLAISIER**, MCX Beamline, Elettra Sincrotrone Trieste, Italy  
*In situ reaction furnace for real-time diffraction studies at MCX@Elettra*
- 15:00-16:30 **MS4: MOLECULAR COMPOUNDS AND INTERMOLECULAR INTERACTIONS**  
Chair: **M<sup>a</sup> Ángeles MONGE**  
  
(Ball Room)
- 15:00-15:30 KN4: **Berta GÓMEZ-LOR**, Instituto de Ciencia de Materiales, Spain  
*Semiconducting triindoles: tuning the crystallographic packing and transport properties through CH- $\pi$  interactions*
- 15:30-15:50 O4.1: **Tommaso NICOLINI**, Politecnico di Milano, Italy  
*Substituted fullerenes in the solid state: phenyl-C61-butyric acid methyl ester and its cocrystals*
- 15:50-16:10 O4.2: **Alessia BACCHI**, Università di Parma, Italy  
*Crystal form landscapes of organometallic catalysts precursors*
- 16:10-16:30 O4.3: **Marta E.G. MOSQUERA**, Universidad de Alcalá, Spain  
*Unusual heterometallic aluminum-alkali metal compounds*
- 16:30-17:00 **Coffee Break**
- 17:00-18:30 **MS5: MEMBRANE PROTEINS AND DRUG DESIGN**  
Chair: **Gianpiero GARAU**  
  
(Oval Room)
- 17:00-17:30 KN5: **Michael HENNIG**, F. Hoffmann – La Roche Ltd., Switzerland  
*Structural biophysics of membrane proteins to facilitate drug discovery*

- 17:30-17:50 O5.1: **Sam Yong PARK**, Yokohama City University, Japan  
*The Structural basis for an essential subunit interaction in influenza virus RNA Polymerase*
- 17:50-18:10 O5.2: **Claudia BINDA**, Università di Pavia, Italy  
*The mitochondrial membrane-bound Monoamine Oxidases A and B drug targets*
- 18:10-18:30 O5.3: **Salvatore BONGARZONE**, Institute for Research in Biomedicine, Spain  
*Structure-driven Development of highly specific Inhibitors against Herpesvirus Terminase*
- 17:00-18:30 **MS6: APERIODIC, NANO-AND DEFECTIVE MATERIALS**  
Chair: **Walter STEURER**  
*(Ball Room)*
- 17:00-17:30 KN6: **Juan Manuel PEREZ-MATO**, Universidad del País Vasco, Spain  
*Compositional uniformity as driving force of nano-patterns: nano-stripes and nano-chessboards*
- 17:30-17:50 O6.1: **Andrea BERNASCONI**, Università di Milano, Italy  
*Local structure of complex industrial glasses: the effect of zinc addition*
- 17:50-18:10 O6.2: **Federica BERTOLOTTI**, Università dell'Insubria and To.Sca.Lab, Italy  
*Silver and copper nitropyrzولاتes: a case of highly defective crystals characterized by the Debye Function Approach*
- 18:10-18:30 O6.3: **Rangana WARSHAMANAGE**, University of Zürich, Switzerland  
*Pushing the limits: determining the average structure in the presence of strong diffuse scattering*
- 18:30-20:00 **RT1: ROUND TABLE ON BIOCRYSTALLOGRAPHY**  
Chair: **Giuseppe ZANOTTI**  
*(Oval Room)*
- 18:30-20:00 **RT2: ROUND TABLE ON GRAPHENE**  
Chair: **Michele SAVIANO**  
*(Ball Room)*

- 18:30-18:40 RT2.O1: **Vittorio PELLEGRINI**, CNR-NANO and Scuola Normale Superiore, Italy  
*Graphene as EU future emerging technology flagship*
- 18:40-18:55 RT2.O2: **Vittorio PELLEGRINI**, CNR-NANO and Scuola Normale Superiore, Italy  
*Prospects for hydrogen storage in graphene*
- 18:55-19:10 RT2.O3: **Camilla COLETTI**, NEST, Istituto Italiano di Tecnologia, Italy  
*Graphene on Cu and SiC substrates: growth and properties*
- 19:10-19:25 RT2.O4: **Elisa MOLINARI**, Università di Modena e Reggio Emilia, and CNR Istituto Nanoscienze, Italy  
*Graphene nanoribbons*
- 19:25-19:40 RT2.O5: **Laura POLLONI**, Università dell'Insubria, Italy  
*Graphene-based technologies*
- 19:40-20:00 Discussion

## Wednesday, September 11<sup>th</sup>, 2013

- 9:00-10:00            **PL3: Carlo GATTI**, INSTM-CNR Milano, Italy  
*Chemical bonding in crystals: charge density and beyond*  
Chair: **Fernando J. LAHOZ**
- 10:00-10:30            **Coffee Break**
- 10:30-12:00            **MS7: QUANTUM CRYSTALLOGRAPHY**  
Chair: **Ángel MARTÍN PENDÁS**  
  
*(Oval Room)*
- 10:30-11:00            **KN7: Julia CONTRERAS-GARCÍA**, Université  
Pierre et Marie Curie, France.  
*NCI: analysis of weak interactions in solids from the electron density*
- 11:00-11:20            **O7.1: Piero MACCHI**, University of Bern, Switzerland  
*Calculation of crystal optical properties from molecular electron density*
- 11:20-11:40            **O7.2: Alessandra FORNI**, Istituto di Scienze e Tecnologie  
Molecolari del CNR and INSTM UdR, Italy  
*New insights into halogen bonding from theoretical approaches and X-ray charge density studies*
- 11:40-12:00            **O7.3: Gianfranco ULIAN**, Università di Bologna, Italy  
*Comparative first-principle investigations of bulk and vibrational properties of phyllosilicate minerals: the case of talc*
- 10:30-12:00            **MS8: INDUSTRIAL, FORENSIC AND HERITAGE  
CRYSTALLOGRAPHY**  
Chair: **Gilberto ARTIOLI**  
  
*(Ball Room)*
- 10:30-11:00            **KN8: Miguel ARANDA**, Universidad de Málaga, Spain  
*From firing ancient potteries to clinkering new eco-cements. Powder diffraction for all-time materials*



- 11:00-11:20 O8.1: **Elisa BARZAGLI**, CNR- Istituto dei Sistemi Complessi, Italy  
*Characterization of an Indian sword, classic and innovative methods of investigation in comparison*
- 11:20-11:40 O8.2: **Volker KALHENBERG**, University of Innsbruck, Austria  
*Structural, spectroscopic and computational studies on a novel microporous thallium silicate*
- 11:40-12:00 O8.3: **Marco FAVERO**, Università degli Studi di Padova, Italy  
*Laboratory in-situ x-ray diffraction and isothermal calorimetry: a useful tool to evaluate cement kinetics*
- 12:00-12:45 **COMMERCIAL PRESENTATIONS #2**  
*(Ball Room)*
- 12:00-12:15 C2.1: **Fraser WHITE**, Agilent Technologies UK Ltd, UK  
*Recent advances in diffractometer software and hardware*
- 12:15-12:30 C2.2: **Jan GERTENBACH**, PANalytical B.V., The Netherlands  
*Extending the capabilities of the multi-purpose Empyrean X-ray diffraction platform*
- 12:30-12:45 C2.3: **Suzanna WARD**, Cambridge Crystallographic Data Centre, United Kingdom  
*New architecture at the CCDC builds foundation for greater insights from crystal structures*
- 12:45-14:00 **Lunch**
- 14:00-15:00 **POSTER SESSION P2: MS4, MS7**
- 15:00-16:30 **MS9: CRYSTALLOGRAPHY AT NON-AMBIENT CONDITIONS**  
Chair: **Giuliana AQUILANTI**  
*(Oval Room)*
- 15:00-15:30 KN9: **Andrzej GRZECHNIK**, Technische Hochschule Aachen, Germany  
*Mixed-valence vanadates at extreme conditions*

- 15:30-15:50 O9.1: **Ewa PATYK**, Adam Mickiewicz University, Poland  
*Compressed stacking in pyrimidine and pyrazine*
- 15:50-16:10 O9.2: **Marco MERLINI**, Università di Milano, Italy  
*New crystal structures of carbonates at Earth's deep mantle condition*
- 16:10-16:30 O9.3: **Rosa Micaela DANISI**, University of Bern, Switzerland  
*In situ dehydration behavior of veszelyite (Cu,Zn)<sub>2</sub>Zn(PO<sub>4</sub>)(OH)<sub>3</sub>·2H<sub>2</sub>O: a single-crystal X-ray study*
- 15:00-16:30 **MS10: CRYSTALLOGRAPHY FOR INTELLIGENT MATERIALS**  
Chair: **Antonia NEELS**  
*(Ball Room)*
- 15:00-15:30 KN10: **Stefan KASKEL**, Technical University of Dresden, Germany  
*New Metal-Organic Frameworks with high porosity and well defined functionality for gas adsorption, separation, and catalysis*
- 15:30-15:50 O10.1: **José Manuel DELGADO LÓPEZ**, IACT (CSIC-UGR), Spain  
*Bioinspired apatite nanocrystals functionalized with monoclonal antibodies for targeted cancer therapy*
- 15:50-16:10 O10.2: **Marco MILANESIO**, Università del Piemonte Orientale, Italy  
*TGA-GC-MS combined with X-ray and electron diffraction to study the degradation, deintercalation, and carbonate contamination in nitrate and organic-exchanged hydrotalcites*
- 16:10-16:30 O10.3: **Olha SEREDA**, CSEM, Switzerland  
*Materials for hydrogen storage: their XRD investigations*
- 16:30-17:00 **Coffee Break**
- 17:00-19:30 **General Assemblies of**  
*(Ball Room)* **AIC**  
*(Oval Room)* **GE3C**  
*(Meeting Room)* **SGK**

20:15 sharp	<b>Departure of buses to Country Restaurant “La Cassinazza” Meeting Point: In front of the Main Entrance to the Football Stadium (next to the Lake Gardens and to the Volta Mausoleum, just across the Carrefour Grocery Store)</b>
20:30	<b>Social Dinner</b>
23:30	<b>Return to Como</b>

## Thursday, September 12<sup>th</sup>, 2013

- 9:00-10:00      **PL4: Sakura PASCARELLI**, ESRF, France  
*Investigating extreme states of matter by x-ray absorption spectroscopy*  
Chair: **Hans-Beat BÜRGI**
- 10:00-10:30      **Coffee Break**
- 10:30-12:00      **MS11: ADVANCES IN CRYSTAL GROWTH AND CRYSTALLIZATION METHODS**  
Chair: **Massimo MORET**  
  
*(Oval Room)*
- 10:30-11:00      **KN11: Francesca P.A. FABBIANI**, Georg-August Universität, Germany  
*Crystallisation and structure determination of imidazolium-based room-temperature ionic liquids*
- 11:00-11:20      **O11.1: Naomi E. CHAYEN**, Imperial College London, United Kingdom  
*Smart materials for protein crystallization*
- 11:20-11:40      **O11.2: Mercedes OSSORIO PERALTA**, Laboratorio de Estudios Cristalográficos, IACT, CSIC-UGr, Spain  
*Experimental study of precipitation and stability of calcium sulfate phases*
- 11:40- 12:00      **O11.3: Raúl BENAGES VILLAU**, Universitat de Barcelona, Spain  
*Growth kinetics of the {10.4} faces of nitratine (NaNO<sub>3</sub>)*
- 10:30-12:00      **MS12: ADVANCES IN POLARIZED X-RAYS AND IN MAGNETIC NEUTRON DIFFRACTION**  
Chair: **Luigi PAOLASINI**  
  
*(Ball Room)*
- 10:30-11:00      **KN12: Emilio LORENZO**, CNRS, France  
*Polarized X-rays and magnetic neutron diffraction: key experiments to unravel complex orders in Nature*

- 11:00-11:20 O12.1: **José Luis GARCÍA-MUÑOZ**, Institut de Ciència de Materials de Barcelona, CSIC, Spain  
*Competing incommensurate magnetic orders and electric polarization in  $Mn_{1-x}Co_xWO_4$  frustrated multiferroics*
- 11:20-11:40 O12.2 **Alessandro BOMBARDI**, Diamond Light Source Ltd., United Kingdom  
*Recent results from X-ray resonant and non-resonant magnetic diffraction on functional materials*
- 11:40- 12:00 O12.3: **Ángel RODRÍGUEZ-FERNÁNDEZ**, Universidad de Oviedo, Spain.  
*Circular polarized resonant X-ray scattering on  $\alpha$ - $Fe_2O_3$  single crystal*
- 12:00-12:45 **COMMERCIAL PRESENTATIONS #3**  
*(Ball Room)*
- 12:00-12:15 C3.1: **Dubravka ŠIŠAK JUNG**, Dectris Ltd., Switzerland  
*Advanced X-ray analysis using single-photon counting detectors*
- 12:15-12:30 C3.2: **Lucia ROBBA**, Bruker Italia S.r.l., Italy  
*High-resolution energy-dispersive one-dimensional detector*
- 12:30-12:45 C3.3: **Stefano CHIESA**, Assing S.p.A., Italy  
*Rigaku diffraction equipment: from scientists to scientists*
- 12:45-14:00 **Lunch**
- 14:00-15:00 **POSTER SESSION P3: MS8,MS9, MS10, MS11, MS12**
- 15:00-16:00 **PL5: Cristobal VIEDMA MOLERO**, Universidad Complutense, Spain  
*Chiral crystallization with nonclassical crystal growth and enantiodiscrimination through oriented attachment*  
Chair: **Catalina RUIZ PÉREZ**

16:00-17:30

**ROUND TABLE ON IYCr 2014**

Chairs: **Fermín OTÁLORA** and **Michele ZEMA**

*(Ball Room)*

17:30

Closing Ceremony