

44th AIC Annual Meeting

14-18 September 2015 Vercelli

Italian Crystallographic Association



UNIVERSITÀ DEGLI STUDI
DI TORINO



We are pleased to announce that in 2015, the XLIV Annual Meeting of the Italian Crystallographic Association (AIC) is held in *Vercelli* by the *Università del Piemonte Orientale A. Avogadro*. The conference is located in the renewed *Complesso Universitario San Giuseppe, Piazza S. Eusebio 5*. [[Interactive Map](#)]

The program, selected by the Scientific Committee, encourages the discussion on emerging methods in crystallography, opening new fields for the investigation of the condensed matter world. Crystal Growth, Nanoscale phenomena, Organic, Inorganic and Biomolecular Systems are studied not only as structural images but also in motion, while working as *Chemical Machines*. Two satellite workshops on emerging topics in materials science [[Program Download](#)] and structural biology [[Program Download](#)] describe new possible ways of exploring the crystallographic world. The numerous Invited lecturers from all Europe, the contribution, also from the scientific viewpoint, of several companies, the Software Fayre and a Round Table on the legacy of the IYCr in Italy further enrich the conference program. [[Full Program Download](#)]

Giuseppe Zanotti-AIC President

Marco Milanese-Chair of Organizing Committee

Scientific Committee

Marco Milanese (Chair); Giuseppe Zanotti (AIC President); Enrico Mugnaioli; Mauro Gemmi; Patrizia Rossi; Silvia Rizzato; Angela Altomare; Antonino Martorana; Alessandro Gualtieri; Dorian Lamba

Organizing Committee

Marco Milanese (Chair); Giovanni Ferraris (Honorary Chair); Simona Galli (Treasurer); Gianluca Croce; Domenica Marabello; Davide Viterbo; Luca Palin; Eleonora Conterposito; Enrico Boccaleri

Steering Committee

Giuseppe Zanotti (AIC President); Michele Saviano; Diego Gatta; Simona Galli ; Annalisa Guerri; Consiglia Tedesco; Michele Zema; Antonietta Guagliardi; Andrea Zappettini; Marco Milanese

603. Crystal-fluid interactions in open-framework materials at high pressure

Paolo Lotti,^a Rossella Arletti,^b G. Diego Gatta,^a

Simona Quartieri,^c Giovanna Vezzalini,^d Marco Merlini^a, Linda Pastero^b

^a*Dipartimento di Scienze della Terra, Università degli Studi di Milano, Milano, Italy*

^b*Dipartimento di Scienze della Terra, Università di Torino, Torino, Italy*

^c*Dipartimento di Fisica e Scienze della Terra, Università di Messina, Messina, Italy*

^d*Dipartimento di Scienze Chimiche e Geologiche, Università di Modena e Reggio Emilia, Modena, Italy*
paolo.lotti@unimi.it

The number of experiments on the high-pressure behavior of open-framework materials increased significantly in the last decade [1,2]. The framework topology, the chemical composition and the so-called “host-guest” interactions (between the framework and the extraframework components) were found to significantly influence the response of zeolites to the applied pressure. However, the HP-behavior of zeolites may also be influenced by crystal-fluid interactions when *P*-transmitting fluids (PTF) are used to generate hydrostatic compression, and in particular when the PTF is “pore-penetrating”. In such a case, the *P*-induced penetration of PTF molecules into the zeolite structural voids leads to a change of the physical-chemical properties of the studied material, for example inducing a stiffening of the elastic behavior or leading to the hyperconfinement of supramolecular aggregates (in the zeolite channels) with functional properties [3].

In this study, we describe the HP-behavior and the crystal-fluid interactions of two synthetic zeolites with empty channels and cages, *i.e.* all-silica ferrierite (Si-FER) and ALPO₄-5 (AlPO₄), compressed with non-penetrating (silicone oil, *s.o.*) and potentially pore-penetrating PTF. The compression of Si-FER in *s.o.* evidences the remarkable flexibility of this framework: a first displacive phase transition was observed from the *Pmnn* to the *P12₁/n1* space group at ~ 0.7 GPa. A second displacive phase transition, involving a significant unit-cell volume contraction, was observed at ~ 1.24 GPa from the *P12₁/n1* to the *P2₁/n11* space group (through an intermediate *P*-1 structure, “type-II” transition according to Christy [4]). The high-*P* *P2₁/n11* polymorph was found to be stable at least up to 3.00(7) GPa, whereas - upon pressure release - the starting *Pmnn* structure was fully recovered. The three polymorphs were found to share a virtually identical bulk elastic behavior, being their average volume compressibility β_V : 0.051(4), 0.056(9) and 0.055(3) GPa⁻¹, respectively. The compression of Si-FER and ALPO-5 in potentially pore-penetrating PTF showed a lower bulk compressibility, different phase-transition paths (for Si-FER) and diverse atomic-scale deformation mechanisms with respect to the compression in silicone oil, suggesting the onset of significant crystal-fluid interactions, likely due to the *P*-induced penetration of PTF molecules. In addition, the HP-behavior of Si-FER is strongly influenced by the process kinetics, which was found to control the *P*-induced molecules intrusion phenomena and, as consequence, the *P*-induced phase transitions in this material.

The authors acknowledge the Italian Ministry of Education, MIUR-Project: “Futuro in Ricerca 2012 - ImPACTRBFR12CLQD”.

[1] G.D. Gatta, Y. Lee *Mineral. Mag.* **2014**, *78*, 267-291. [2] G. Vezzalini, R. Arletti, S. Quartieri *Acta Cryst.* **2014**, *B70*, 444-471. [3] M. Santoro, F.A. Gorelli, R. Bini, J. Haines, A. Van der Lee *Nat. Commun.* **2013**, *4*, 1557-1563. [4] A.G. Christy *Acta Cryst.* **1993**, *B49*, 987-996.

INDEX

Introduction

GOLD MEDAL MARIO MAMMI - Things Done and Things Yet To Be Done: Crystallography at Large, 2015-2030

MARIO NARDELLI PRIZE - Crystal Engineering on “Tailor-Made” Multifunctional Zirconium Phosphonates

PhD's THESIS AWARD in CRYSTALLOGRAFY - New Forms of Polar and Spin Ordering in Pb₂(Mn,Co)WO₆ Double Perovskites: Symmetry Analysis of Ferroic Properties

PLENARY LECTURES

PL.1 New Advances in Electron Diffraction: from Ab-initio Structure Solution to Refinement

PL2. Ab-initio Modeling in Crystallography

PL3. Watching Matter in Motion: Time Resolved Studies from Synchrotrons to FELs

PL4. Electron Diffraction and Imaging of Protein and Pharmaceutical 3D Nanocrystals

MICROSYMPOSIA

* MS1. Advanced Theoretical and Experimental Methods in Crystallography

1KN1. Advances in methods for macromolecular structure solution: ab initio and MR approaches

1KN2. Advances in microstructure analysis of materials with defects

1O1. Quantum Mechanical Simulation Of Protein Crystals: The Case Of The Small Protein Crambin

1O2. Experimental and theoretical charge density study of iodoperfluoroalkylimidazoles self-assembled through halogen bond

1O4. Structural characterization of LDH samples by ADT and TGA-GC-MS: thermal response and contamination in nitrate and organic-exchanged hydrotalcites

1O5. Polymer Brushes and Their Composites with Silver Nanoparticles: An X-Ray Reflectivity and Positron Annihilation Spectroscopy Study

1P1. Modelling The Carbonate Substitution In Hydroxyapatite Towards Bone Composition

1P2. Chemical selectivity in structure determination by time dependent analysis of in situ XRPD data: a clear view of Xe thermal behavior inside a MFI zeolite

1P3. New advances of QUALX2.0, a qualitative phase analysis software querying a freely available database

* MS2. Investigating Structure-Property Relationships in Complex Molecular Systems by a Multi-Technique Approach

2KN1. New insight into the properties of indomethacin pharmaceutical co-crystals

2KN2. Biomolecules as ligands to construct high-dimensional coordination networks (bioMOFs): towards a rational design of more feasible biocompatibility and homochiral materials

2O1. Molecular Rotors in Porous Covalent Frameworks and Supramolecular Architectures

2O2. Characterization of the solid state dynamic behaviour of cyclic peptoids

2O3. Promising Low-Dielectric-Constant Materials: Metal-organic Frameworks and Coordination Polymers Compared

2O4. Fifty Years of Sharing Crystal Structures

2P1. Homochiral Self-Assembly of Biocoordination Polymers: Anion-Triggered Helicity and Absolute Configuration Inversion

2P2. Naphthalene diimide cocrystals based on halogen bond

2P3. From crystallography to applications: non linear optical properties of β -D-fructopyranose alkaline halides MOFs

2P4. Studies of the conformational changes on the ribosomal GTPase EFL1 using SAXS

2P5. Stacking motives in metallate salts of methylene blue

* MS3. From Nature to Advanced Materials: Structure Characterization at the Nanoscale

3KN1. Rotation electron diffraction as a complementary technique to powder X-ray diffraction for phase identification and structure solution

3KN2. How difficult is to solve complex structures: the case of Eni Carbon Silicates

3O1. 3D Investigation of the Reciprocal Space of Nano-Crystals by Electron Diffraction Tomography

3O2. Structure determination using ab-initio methods and simulated annealing from PED tomography

3O3. Organized architecture of dyes in zeolite channels: an effective transport of electronic excitation energy

3O4. Structural evolution of tungsten oxide nanocrystals investigated by Pair Distribution Function and Modulation Enhanced Diffraction

3P1. Electron diffraction study of polyphasicnanocrystalline $M_2O-Al_2O_3-WO_3$ ($M = Na, K$) system

3P2. Average and Local structural comparison of $BaTi_{1-x}Ce_xO_3$ by Pair Distribution Function

3P3. Photocatalytic Shaping of Silver Nanoprisms Self-Assembled on Anatase Thin Films

* MS4. New Topics in Crystal Growth Research

4KN1. Uncovering the role of solvent in organic crystals nucleation and growth

4KN2. The role of the adhesion energy in surface and interface growth processes: apatites and alkali-halides.

4O1. Turning liquid drugs into crystals

4O2. Exploiting dimensional variability in coordination polymers: solvent promotes reversible conversion between 3D and chiral 1D architectures

4O3. Catalyst-free vapour-phase growth of Ga_2O_3 nanowires and nanobelts

4O4. New Fluorinated Metal-Organic Frameworks Self-Assembled via Halogen Bonding

4P1. Cu₂-xS ultra thin films obtained by electrodeposition: a structural characterization

4P2. Recrystallization behavior of amorphous venlafaxine free base prepared by melt technique

4P3. A computational approach to the study of epitaxy

4P4. Facile intercalation of organic molecules into hydrotalcites by liquid assisted grinding: yield optimization by a chemometric approach

4P5. New Co-crystals of Salicylic acid: from screening to synthesis and structural characterization

4P6. Morphological and Structural Effects of Gels on Coordination Polymers Crystallization

* MS5. Nanostructures and Nanoscale Phenomena

5KN1. Characterization of nano-structured materials by synchrotron radiation techniques

5KN2. Application of Total Scattering Methods to the Investigation of Clean Energy Materials

5O1. Disclosing the Rhombohedral Structure of Colloidal Lead Chalcogenides Quantum Dots, their stoichiometry and their shape evolution through the Debye Function Analysis

5O2. Spatially resolved photoemission spectromicroscopy: a powerful tool for the characterization of nanostructured novel materials.

5O3. microEXAFS and microXANES for the study of Solid Oxide Fuel Cells

5P1. A super cell approach for the refinement of carbonate hydrotalcites affected by stacking faults

5P2. Stress measurements at the nanoscale by ZnO Nanorods-modified Carbon Fibers

5P3. The DebUsSy Suite 2.0: a powerful tool for characterizing nanosized materials through the Debye Scattering Equation

5P4. Core-shell cobalt/cobalt oxide nanoparticles: a Debye function XRD pattern simulation

* MS6. Crystal Chemistry of Inorganic Compounds for the Understanding of Their Properties and Stability

6KN1. Time for Changes: Nanosized Magnetite Clusters on the Run

6KN2. Tracking structural and electronic properties of coordination compounds: the role of synchrotron radiation

6O1. Adsorption/Desorption Of Fuel Based Pollutants Confined within ZSM-5: a Combined In Situ High-Temperature Synchrotron Powder X-Ray Diffraction and Chromatographic Study

6O2. After a century of Bragg diffraction, how well do we know the structures of inorganic compounds?

6O3. Crystal-fluid interactions in open-framework materials at high pressure

6O4. In situ high-temperature X-ray diffraction and spectroscopic study of fibroferrite, FeOH(SO₄)×5H₂O

6O5. Structural characterization of magnetoresistive Pb₂FeMoO₆

6P1. Twinning: structural peculiarities and opportunities in coordination polymers

6P2. Improper Ferroelectric state in a double perovskite system with a collinear magnetic structure

6P3. CO2 adsorption in Faujasite systems: a synchrotron X-Ray Powder Diffraction investigation

6P4. Crystallographic and chemical transformation of asbestiform erionite and chrysotile asbestos in cell environment

6P5. Compressibility and high-pressure behaviour of lead feldspar

6P6. Alkali activated materials from sulfate-bearing kaolins: pros and cons

* MS7. Imaging Biomolecular Machines in Action through Cryo-Electron Diffraction and Cryo-Electron Microscopy

7KN1. The atomic structure of the human gamma-secretase complex

7KN2. Molecular mechanisms of asymmetric cell divisions

7O1. Membrane NAPE-PLD links major players in lipid homeostasis with major players in lipid mediated signaling

7O2. Pore flexibility underlies the poor selectivity of CNG channels: a structural, functional and computational analysis

7O3. Have your phosphate and eat it: structure and function of a bacterial PhoX phosphatase

7O4. How to build a host-parasite interactome: a proof of concept for Schistosoma mansoni

7P1. Platinum binding to human copper chaperone Atox1

7P2. Single-particle cryo-EM study of the AMPA receptor in the desensitized state

7P3. Three-dimensional structure and ligand-binding site of carp Fischelectin (FEL)

7P4. Structural studies of human acidic fibroblast-growth factor (FGF1) mutants with a probable anticancer activity

7P5. Unraveling the antitumoral properties of Arundo donax lectin

7P6. Structural Characterization Of Proteins Involved In Helicobacter pylori Motility And Adhesion

7P7. Multi-Target-Directed Ligands in Alzheimer's Disease Treatment

7P8. The Structure of the T190M Mutant of Murine α -Dystroglycan at High Resolution: Insight into the Molecular Basis of a Primary Dystroglycanopathy

7P9. A PPP Platform at Elettra: achievements and future perspectives

* MISCELLANEOUS

MP1. Crystal Structure of Functionalized Croconaines

* SOFTWARE FAYRE

The EXPO program

The SIR program

The CRYSTAL program

ROUND TABLE - The Future of Crystallography and the Legacy of IYCr in Italy

* COMMERCIAL PRESENTATIONS

Progress in X-ray Crystallographic Methodology: Shutterless Data Collection

XRPD Solutions to Industrial Application Fields