44 AIC Annual Meeting

14 -18 September 2015 Vercelli

Italian Crystallographic Association

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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]

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

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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 H*P*-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 H*P*-behavior and the crystal-fluid interactions of two synthetic zeolites with empty channels and cages, *i.e.* all-silica ferrierite (Si-FER) and $ALPO_4$-5 ($AlPO_4$), 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 $P12_1/n1$ 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 $P12_1/n1$ to the $P2_1/n11$ space group (through an intermediate *P*-1 structure, "type-II" transition according to Christy [4]). The high-*P* $P2_1/n11$ 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 H*P*-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.

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[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

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