Report on the MISSCA 2013 International Crystallographic Conference

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Early in September 2013, only a few months away from the International Year of Crystallography (2014), nearly 230 scientists from more than 15 different Countries gathered in Como, for an International Conference co-organized by the Italian, Spanish, and Swiss Crystallographic Associations, presenting their most recent crystallographic results in variety of fields, in basic and applied Science. This brief account highlights the topics discussed during the conference, and the future of the European crystallographic research, with its relevance to distinct fields of physics, chemistry, biology, materials, and earth science, as well as in preservation of cultural heritage.
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UNESCO has recently resolved that Year 2014 will be devoted to the celebrations of the International Year of Crystallography. Accordingly, the Italian, Spanish, and Swiss Crystallographic Associations (see Figure 1), following a recent tradition of joint Conferences [2007, Copannello di Stalettì (Italy); 2010, Oviedo (Spain)], decided to co-organize a larger event, that is an International Conference (MISSCA – Meeting of the Italian, Spanish, and Swiss Crystallographic Associations), which took place early in September 2013 in the beautiful surroundings of the 18th Century Villa Olmo in Como. The choice of this location was also catalyzed by the presence, in Como, of several crystallographers from the University of Insubria and the Istituto di Cristallografia of the Italian CNR, who enthusiastically provided many young helpers necessary for a successful realization of such an event. Of the nearly 200 contributions presented during the whole of the Conference (lasting 4 days), 5 were plenary lectures, 60 were oral presentations (including 12 keynotes) and more than 100 were posters.

PLENARY LECTURES

Five plenary lectures of extremely high quality have clearly manifested the relevance of disseminating crystallographic techniques within fields of relevant scientific and technological importance.

Stuart Parkin (IBM Almaden Research Center, San José, USA) gave a fascinating talk, entitled Turning insulators into metals!, in which transition metal oxides, in the presence of high electric fields and in the presence of ionic liquids, were shown to dramatically change their electrical conductivity properties, opening the way to new (fast and low power) methods for storing or transporting information. Later, Tilman Schirmer (University of Basel, Switzerland) presented, in Mechanisms to regulate the cellular concentration of the bacterial second messenger c-di-GMP, the molecular mechanisms governing the synthesis and the degradation of the second messenger c-di-GMP, characterized by advanced structural and functional biology methods. On the 3rd day, Carlo Gatti (ISTM-CNR, Milan, Italy) gave a plenary lecture entitled Chemical bonding in crystals: charge density and beyond, highlighting the theoretical basis, the historical development, and several paradigmatic examples of the physico-chemical interpretation of structural anomalies, using the formalism of topological partitioning. The last day benefitted from two distinct plenary lectures: Sakura Pascarelli (ESRF, Grenoble, France), on Investigating extreme states of matter by X-ray absorption spectroscopy, and Cristobal Viedma-Molero (Universidad Complutense, Madrid, Spain), on Chiral crystallization with nonclassical crystal growth and enantiodiscrimination through oriented attachment; Pascarelli enchanted the audience by reporting on innovative experiments on metals and metal oxides under extremely high pressures, mimicking chemical reactions occurring in the Earth's core and investigating the modulation of magnetic properties of materials of high technological impact; Viedma Molero described spontaneous enantioselective processes during collective recrystallization mediated by nanostructured clusters or even by crystals of micro- or millimeter size.

THEMATIC MICROSYMPOSIA

During the MISSCA Conference, several crystallography-related topics have been tackled within 12 microsymposia (see Figure 2), which were characterized by the following titles:

MS1 – Macromolecular Assemblies and Viruses,
MS2 – Structure and Properties of Organic and Inorganic Thin Films,
MS3 – Frontiers in Instrumentation,
MS4 – Molecular Compounds and Intermolecular Interactions,
MS5 – Membrane Proteins and Drug Design,
MS6 – Aperiodic, Nano- and Defective Materials,
MS7 – Quantum Crystallography,
MS8 – Industrial, Forensic and Heritage Crystallography,
MS9 – Crystallography at non-Ambient Conditions,
MS10 – Crystallography for Intelligent Materials,
MS11 – Advances in Crystal Growth and Crystallization Methods,
MS12 – Advances in Polarized X-rays and in Magnetic Neutron Diffraction.

Figure 1. The symbols of the Italian, Swiss, and Spanish Crystallographic Associations and that of the guest institution, University of Insubria.

Within the long list of contributions given in these sessions, several keynote presentations were given: Maria Solà (IBMB-CSIC, Barcelona, TFAM: a highly flexible system to modulate mitochondrial DNA); Frank Schreiber (Eberhard Karls Universität, Tübingen, Real-time X-ray scattering studies of thin film growth); Ian K. Robinson (London Centre for Nanotechnology, Opportunities for coherence in crystallography); Berta Gómez Lor (Instituto de Ciencia de Materiales, Madrid, Semiconducting triindoles: tuning the crystallographic packing and transport properties through CH-π interactions); Michael Hennig (Hoffmann – La Roche Ltd., Basel, Structural biophysics of membrane proteins to facilitate drug discovery); Antonio Cervellino (Paul Scherrer Institut, Villigen, Structure, microstructure and surface superstructure of magnetite/maghemite nanoparticles); Julia Contreras-García (Université Pierre et Marie Curie, Paris, NCI: analysis of weak interactions in solids from the electron density); Miguel A.G. Aranda (Universidad de Malaga e CELLS-ALBA, Barcelona, From firing ancient potteries to clinkering new eco-cements. Powder diffraction for all-time materials); Andrzej Grzechnik (Technische Hochschule, Aachen, Mixed-valence vanadates at extreme conditions); Stefan Kaskel (Technische Universität Dresden, New Metal-Organic Frameworks with high porosity and well-defined functionality for gas adsorption, separation, and catalysis); Francesca P.A. Fabbiani (Georg-August Universität, Göttingen, Crystallisation and structure determination of imidazolium-based room-temperature ionic liquids); Emilio Lorenzo (ESRF, Grenoble, Polarized X-rays and magnetic neutron diffraction: key experiments to unravel complex orders in Nature) (see Figure 3).

Among the other oral presentations, in a non-exhaustive list, we highlight hereafter those who, in our opinion, have greatly attracted the interest of the Conference audience: Evelyn Moreno-Calvo (Institut de Ciència de Materials, Barcelona, Quatsomes: vescicular structures formed by self-assembly of sterols and quaternary ammonium surfactants); Fabiola Liscio (IMEM-CNR, Bologna, Control of octathiophene fibers orientation fabricated by lithographically wetting

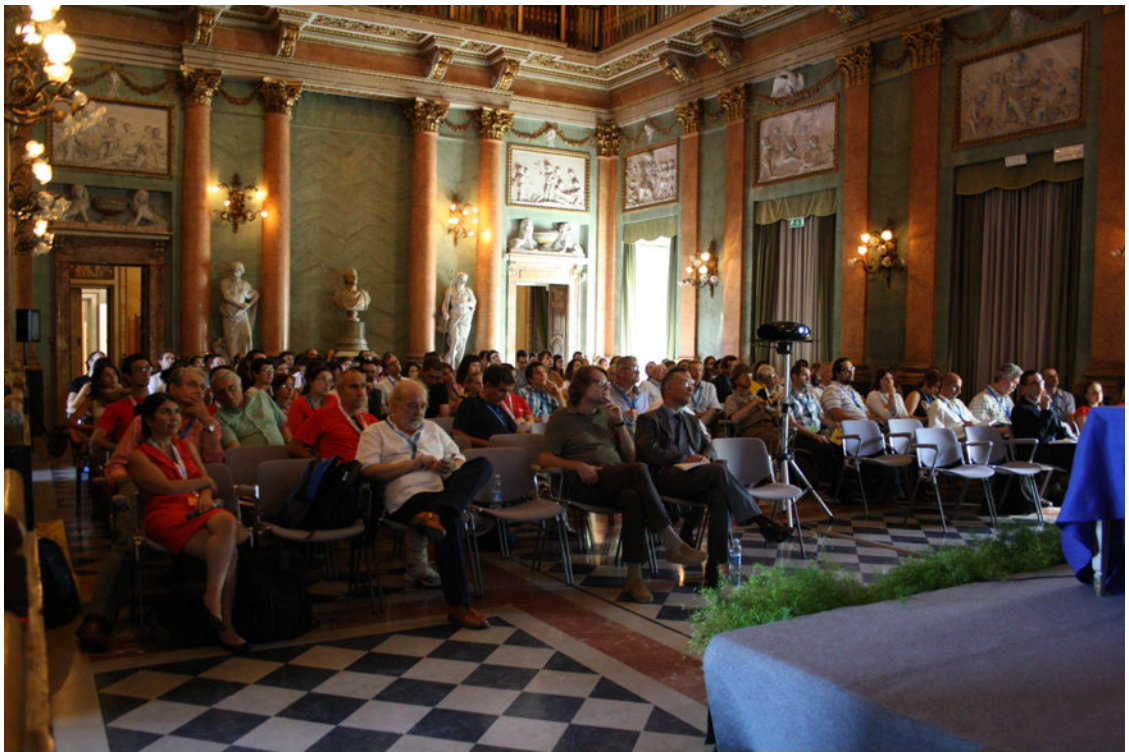

Figure 2. Attendees at one of the many microsymposia of the MISSCA Conference.

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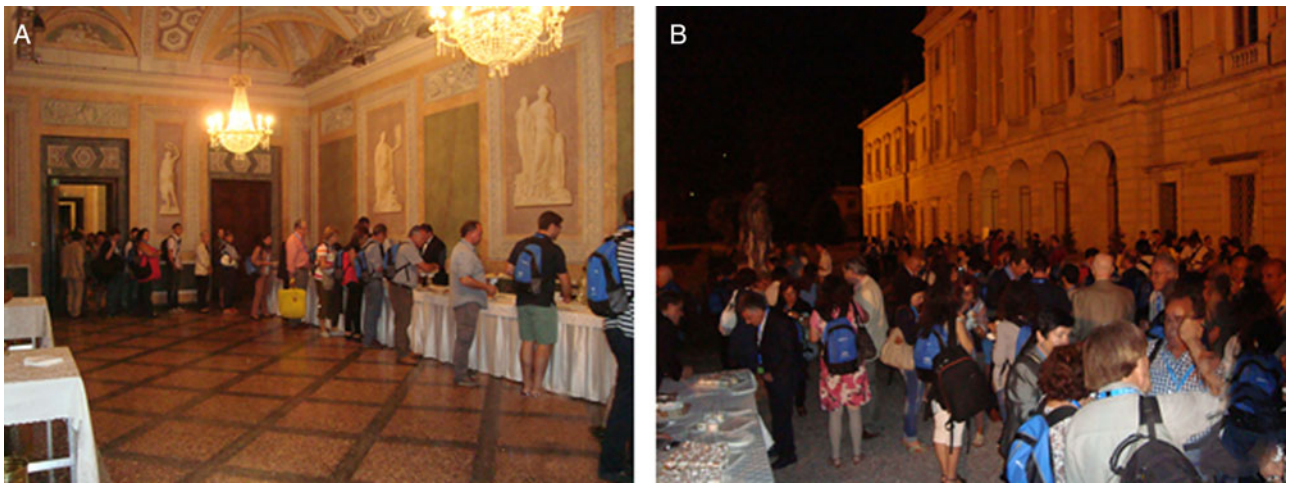

Figure 3. Real example of an irreversible order–disorder transition.

process); Jürg Schefer (Paul Scherrer Institut, Villigen, HEIMDAL: a time-of-flight neutron powder diffractometer going beyond today's designs by offering additionally a SANS and an imaging option); Alessia Bacchi (Università di Parma, Crystals form landscapes of organometallic catalysts precursors); Sam Yong Park (Yokohama City University, The structural basis for an essential subunit interaction in influenza virus RNA Polymerase); Federica Bertolotti (Università dell'Insubria e To.Sca.Lab, Como, Silver and copper nitropyrazolates: a case of highly defective crystals characterized by the Debye Function Approach); Piero Macchi (Universität Bern, Calculation of crystal optical properties from molecular electron density); Ewa Patyk (Uniwersytet Adama Mickiewicza, Poznań, Compressed stacking in pyrimidine and pyrazine); José Manuel Delgado López (IACT-CSIC, Granada, Bioinspired apatite nanocrystals functionalized with monoclonal antibodies for targeted cancer therapy); Naomi E. Chayen (Imperial College London, Smart materials for protein crystallization); Olha Sereda (Centre Suisse d'Electronique et Microtechnique, Neuchâtel, Materials for hydrogen storage: their XRD investigations); Alessandro Bombardi (Diamond Light Source Ltd., Recent results from X-ray resonant and non-resonant magnetic diffraction on functional materials).

OTHER TALKS

As in other occasions, several prestigious prizes have been assigned to different awardees for their scientific activities: from undergraduate and graduate students, up to internationally renowned scientists. Among these prizes, that honoring the memory of Professor Nardelli (University of Parma), assigned to the young researcher Laura Cendron (University of Padua, Structural and functional studies on HydF, an enzyme with a key role in the maturation of the [FeFe]-hydrogenase catalytic core); the "career" prize (honoring the late Prof. Mammi, University of Padua), assigned to Roberta Oberti (IGG-CNR, Pavia, Chipping, baking, and squeezing amphiboles (and more): the importance of crystal-chemical models); the MISCA Gold Medal to Juan Manuel García Ruiz (IACT-CSIC, Granada), who presented a very interesting and charming plenary lecture entitled Crystals and (my) life.

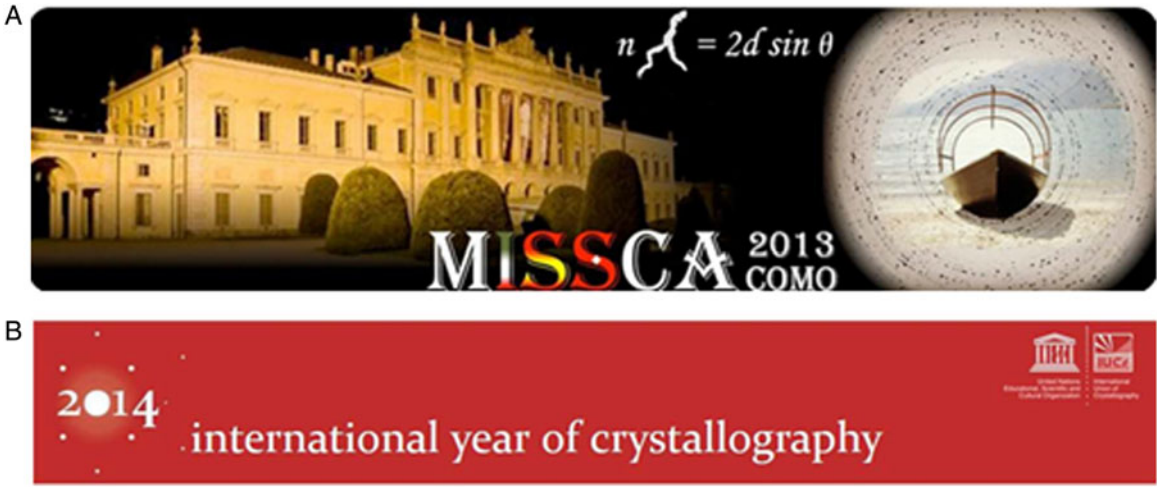

Figure 4. (A) top: the logo of the MISSCA 2013 Conference (with the Lake of Como shape inserted in Bragg's equation). (B) bottom: the banner of the International Year of Crystallography.

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Not to be forgotten, three special sessions on specific and timely themes were organized with the constant participation of the whole audience with topical presentations and open discussions on the present and the future of three different subjects of extreme importance, for their scientific, applied and educational aspects: a round table on biocrystallography, organized by Giuseppe Zanotti (University of Padua) and Armando Albert (IQC-CSIC, Madrid); one centered on graphene, moderated by Michele Saviano (IC-CNR, Bari); and one on the events to be organized by the three crystallographic Societies to celebrate the International Year of Crystallography, coordinated by Michele Zema (International Union of Crystallography and University of Pavia) and Fermín Otálora (IACT-CSIC, Granada).

Significantly, many commercial sponsors have also actively participated to the Conference, and were given also the opportunity to present their most recent products and methodological developments to an interested audience, thanks to the organization of dedicated sessions.

SUMMARY

In conclusion, the topics covered in the different contributions attest to the liveliness and the multidisciplinary character of crystallography in very distinct fields, with relevant fall-out in a number of applied fields: from nanotechnologies (organic electronics; solid state memories and drug delivery), to important and widely spread goods and commodities (cements, glasses, and batteries), to life sciences (drugs, proteins, tissue engineering, and regenerative medicine) and earth sciences (mineralogy and petrography) and environment and cultural heritage protection and preservation.

In particular, the academic or industrial origin of the different speakers, coming from well beyond the borders of the three countries co-organizing the MISSCA 2013 Conference, has allowed the growth of a scientific and cultural event which reached a truly European level (if not further). Therefore, this Conference has opened the International Year of Crystallography [see Figures 4(A) and 4(B)] with a keen anticipation of the long series of events (to be soon) globally organized at the National and International levels. All together, these events will likely manifest a specific educational character, being addressed to high-school and college students, as well as to the laymen: workshops, meetings, and educational pamphlets will be organized, such as the itinerant exhibition named CRISTALLI! which, initially located in the University Museum of the University of Padua, will soon tour throughout Italy, North to South, in the cities of Como, Modena, Firenze, Napoli, and Cosenza.

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