

4 Joint AIC - SILS Conference



Monday 12 September 2022 - Thursday 15 September 2022

Scientific Programme

Modern Integrative Structural Biology

****Chairs: S. Mangani, B. Vallone****

The complexity of the chemistry occurring in living organisms involves interactions between large numbers of a variety of molecules. In order to achieve a better understanding, at the structural level, of the processes occurring in the crowded environment of cells there is need to exploit the capabilities of different experimental techniques. Modern Integrative Structural Biology addresses this subject and involves cross-links of data coming from X-ray crystallography, cryo-electron microscopy/tomography, computational methods, NMR, XAS, SAXS and other spectroscopies to produce structural models of biological systems.

The microsymposium aims to highlight updated scientific results obtained by such integrated approaches.

Understanding Advanced Functional Materials Through Operando Studies

****Chairs: E. Borfecchia, S. Galli****

The microsymposium will focus on in situ/operando studies aimed at disclosing the structural and physico-chemical properties of advanced materials and at tracking their response in controlled environments relevant to the target functional application. An emphasis will be given to cutting-edge diffraction methods applied under non ambient conditions and synchrotron-based X-ray spectroscopies exploiting in situ/operando setups, as well as to their possible combination and integration within multi-technique approaches. The microsymposium is envisaged to encompass a broad range of high-impact research fields, including, e.g., (photo/electro-) catalysis, gas adsorption and separation, energy storage and conversion.

Italy@EuXFEL

****Chair: S. Pascarelli****

The European X-Ray Free-Electron Laser (EuXFEL) provides the international user community hard and soft x-ray flashes with unprecedented characteristics, enabling new experiments in a variety of scientific fields ranging from condensed matter physics to chemistry and from geophysics to biosciences. In 2020, in synergy with SILS, EuXFEL initiated an effort to better organize its scientific exploitation by Italy and a first very successful "Italy@EuXFEL 2020" workshop demonstrated the interest by the scientific Italian community to take advantage of the unique features of EuXFEL. At this MS, first results in particular from Italian users will be presented, and discussions will focus on how to foster tighter links between EuXFEL and potential Italian users.

Frontiers in Mineralogy and Inorganic Geochemistry

****Chairs: D. Belmonte, G. Giuli****

This microsymposium deals with state of the art techniques (using either laboratory facilities or

synchrotron light sources) aimed at studying structure, chemistry, reactivity, thermodynamic and physical properties of minerals, glasses, melts and fluids of interest in Earth Science and technological applications.

We encourage submission of contributions reporting advanced experimental and/or numerical approaches aimed at studying mineralogical and geochemical aspects related to both Earth Science and advanced technology.

Experimental Design & Analysis of Data

****Chair: M. Milanesio****

The recent evolution of both sources and detectors allowed improving the data quality and signaling to noise ratio at XFEL, synchrotron and laboratory X-ray sources. X-ray diffraction and spectroscopy techniques can now be carried out routinely at high resolution with a time frame of seconds or even much less with a high degree of automation in sample manipulation and experiment execution. New experimental possibilities and new challenges are emerging. Innovative methods, complementary to traditional ones, are necessary to face “the X-ray big data” analysis and propose efficient solutions. The microsymposium is focused on the new avenues of both methods and data analysis in X-ray diffraction and spectroscopies of the XXI century.

Crystallographic and Spectroscopic Advanced Tools Applied to Pharmaceuticals

****Chair: F. Gozzo****

This microsymposium is intended to be the opportunity for academic and industrial scientists to exchange on the main challenges faced in the pharmaceutical world and the advanced methodology available for the characterization of pharmaceutical compounds. The microsymposium welcomes contributions dealing with the many aspects related to the advantages offered by the combination of different characterization methods applied to pharmaceuticals.

Materials at Extreme Conditions: X-ray Crystallography and Beyond

****Chairs: G. Aquilanti, D. Comboni****

In the last decades, experiments at non-ambient conditions have greatly benefited from the improvement of large-scale facilities, which allow investigating and manipulating matter at extreme PT conditions. Experiments performed at non-ambient conditions are devoted to unveil the interplay between structure, physical properties, reactivity and the deformation mechanisms of various materials, expanding our knowledge regarding the evolution of planets and providing critical information to tailor the future new cutting-edge materials. This microsymposium aims to be the stage for scientists who wish to show the results of their research performed under extreme conditions using a variety of analytical techniques.

Bright Radiation Sources and Novel Software Applications

****Chairs: C. Cuocci, F. Stellato****

AIC and SILS societies collect scientists exploiting high intensity photons and electron beams to study a wealth of crystalline and non-crystalline systems. The microsposium dedicated to “Bright Radiation Sources and Novel Software Applications” acts as a bridge connecting the two sides of the research.

On the one hand, the microsposium collects contributions about the brightest present and future radiation sources, keeping an eye on the new experiments they will allow. On the other hand, it hosts talks describing the most recent software developments that allow an increasingly efficient information extraction from the experimental measurements.

Current Approaches in Structural Biology

****Chairs: M. Cianci, S. Fermani****

In the last decades, structural biology has experienced a tremendous growth. The ensemble of low- and high-resolution techniques now available offers the possibility of studying complex macromolecular structures at an unprecedented resolution. Historically, X-ray crystallography was the preferred method for structure determination; however, alternative/complementary approaches are further increasing our capability to explore previously intractable molecules. This microsposium is focused on the current strategies (single or in combination) used to study both the structure and the dynamics of proteins and protein complexes which are relevant for biomedical and biotechnological applications.

Investigating Molecular Crystals: Methods and Applications

****Chairs: A. Forni, E. Priola****

This Microsposium welcomes contributions from both fundamental and applicative research on solid-state molecular systems, where knowledge of the crystal structure, possibly combined with information obtained from quantum mechanical calculations, is vital to understand properties, processes and reactivity. Examples include, but are not limited to, quantum crystallography studies on molecular properties and intermolecular interactions, structure/properties investigations on emissive and non-linear optical materials, crystal engineering of functional materials.

Interplay between Crystal Growth and Advanced Characterizations for Materials Development

****Chairs: F. Boscherini, P. Prete****

To go beyond a trial and error approach for the optimization of functional properties of modern materials a close connection between the development of novel methods for crystal growth and use of refined tools for their experimental characterization is essential. The goal of this interplay is to gain a physical understanding at the atomic level of materials properties. In this symposium we aim to highlight recent results in these two strongly connected and challenging areas of materials science.

Nanostructured Materials

****Chair: P. Scardi****

The study of materials at the nanoscale is now an integral part of various research disciplines, which go far beyond materials science and concern all the physical, chemical and life sciences. Diffraction and imaging techniques, in particular those based on X-rays, are among the most widespread tools both in basic research and in the development of applications of nanostructured materials. The microsymposium aims to collect the state of the art in crystallography and X-ray analysis applications in this lively and ongoing field of research.

Science & Society: from Dissemination to Communication

****Chairs: P. D'Angelo, M. Morana****

Crystallography and synchrotron radiation are fascinating topics that play a major role in a wide range of disciplines, shedding light on materials, minerals, and biomolecules. However, the general public is mostly unaware of this contribution. This microsymposium aims to promote dissemination and outreach of these themes, highlighting the importance of science communication in many different aspects of everyday life, including the ongoing COVID-19 pandemic. At the same time, we want to stimulate the discussion about the interplay between science and society in terms of inclusion, representation and diversity.