1st National Congress of the Mexican Society of Synchrotron Light & 1st International Congress of Synchrotron Light Techniques

Monday 21 June 2021 - Saturday 26 June 2021

León, Guanajuato

SOCIEDAD MEXICANA
DE LUZ SINCROTRÓN A.C.

Book of Abstracts

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The Board of SMLS has published the call to its 1st National Congress of the Mexican Society of Synchrotron Light and the 1st International Congress of Synchrotron Light Techniques to be virtually held from June 21th to 26th, 2021 in Leon, state of Guanajuato, México.

PRESENTATION

Today, modern research uses radiation synchrotron techniques. These play an important role in research being carried out in many universities and research centers around the world.

In our country, these techniques are used for front-line research and are used in innovative technologies. These techniques are used in a variety of areas of science, such as biology, chemistry, materials science, geology, cultural heritage, physics, medicine and life sciences.

This event will consist of plenary lectures, conferences, technical presentations, oral and poster presentations. Fundamental and advanced courses on synchrotron light techniques will be given simultaneously.

APPLICATION AREAS OF SYNCHROTRON RADIATION

Areas where synchrotron light is used include biology, chemistry, materials sciences, geology, cultural heritage, physics, medicine, and life sciences, among others.

Contents

Contribution ID : **1** Type : **Presentation**

CRYO-EM: THE STRUCTURE AND DYNAMICS OF BIOMOLECULES IN THEIR NATIVE STATES

Monday, 21 June 2021 09:30 (1:30)

Abstract

The aim of Structural Biology is to explain life processes in terms of macromolecular interactions in the cell. These interactions typically involve more than two partners, and can run up to dozens. A full description will need to characterize all structures on the atomic level, and the way these structures change in the process. Because of the crowded environment of the cell, such characterization is presently only possible when the group of interacting molecules (often organized into processive “molecular machines") is isolated and studied in vitro. While X-ray crystallography has provided structures of a large number of molecular structures, the need for crystals diffracting to high resolution has severely limited the number of supramolecular assemblies and the range of conformers that can be studied with this technique. Single-particle cryo-electron microscopy is about to fill this gap, allowing fụnctional processes to be studied in great detail without imposing restraints on the structures. There are many examples now for this expansion of Structural Biology toward a full characterization of a functional process. Future developments of single-particle cryo-EM include the study of short-lived intermediates in a nonequilibrium system by time-resolved techniques, and the characterization of continuous structural changes using data mining from large ensembles of molecule images.

About

Joachim Frank is a German-American biophysicist at Columbia University and a Nobel laureate. He is regarded as the founder of single-particle cryo-electron microscopy (cryo-EM), for which he shared the Nobel Prize in Chemistry in 2017. He has also made significant contributions to structure and function of the ribosome from bacteria and eukaryotes.

Primary author(s) : Dr. FRANK, Joachim (Department of Biochemistry and Molecular Biophysics, Columbia University.)

Presenter(s) : Dr. FRANK, Joachim (Department of Biochemistry and Molecular Biophysics, Columbia University.)

Session Classification : Keynote Speech

Contribution ID : **2** Type : **Presentation**

SCIENCE IN MÉXICO WITH AND WITHOUT A SYNCHROTRON LIGHTSOURCE

Monday, 21 June 2021 11:30 (1:00)

Abstract

An overview of the initiative to establish an Advanced Light Source in Mexico in the last two decades is presented. The technical, political and economic challenges that this project needs to overcome are summarized. So far, the last four federal administrations have had a variety of responses and answers to our proposal. Yet a handful high level politicians have endorsed the project, the most recent of them is the present governor of Mexico´s Hidalgo State. Based on a critical assessment of the successes and shortcomings of the actions so far taken by the scientific and technical community, I suggest a road map required to accomplish this indispensable infrastructure. I will use an improbable analogy of the Mexican Synchrotron Scientific Community endeavors with the 2020 Nobel Physics´ Prize.

About

El Dr. Fernando Matías Moreno Yntriago obtuvo su Licenciatura, Maestría y Doctorado en Fisica por la Facultad de Ciencias de la UNAM. Es Profesor-Investigador de Tiempo Completo en el Instituto de Física de la UNAM desde 1985. Ha realizado diversas estancias sabáticas en Centros Internacional, como es el Centro Internacional de Fisica Teórica en Trieste, Italia y en la Universidad Católica de Louvain en Bélgica. Ha sido distinguido con la medalla de la División de Particulas y Campos que otorga la Sociedad Mexicana de Física. Realiza investigaciones en física de altas energías en aplicaciones de la radiación sincrotrónica.

Primary author(s) : Dr. MORENO, Matías (Instituto de Física, UNAM)

Presenter(s) : Dr. MORENO, Matías (Instituto de Física, UNAM)

Session Classification : Plenary Lecture

Contribution ID : **3** Type : **Presentation**

STATUS AND PERSPECTIVES OF ELETTRA AND FERMI

Monday, 21 June 2021 12:30 (1:00)

Abstract

Despite the COVID-19 pandemic the Elettra synchrotron radiation source and the FERMI free-electron laser were able to continue operation without any interruption. The reduced mobility of European users, however, has substantially affected the number of proposed experiments that could be carried out. Increased reliance on sample mail-in with experiments carried out by the facility staff for the external users coupled with enhanced capabilities for data communication and remote operation of the instrumentation were used to reduce the impact, but approximately 56% of the user beamtimes in 2020 had to be postponed.

In 2020 the Elettra source operated with 97% efficiency with 28 beamlines and experimental stations open to international users. Important upgrades have been performed on several beamlines. As examples, we mention the new energy analyzer of the Spectroscopic PhotoEmission and Low Energy Electron Microscope of the Nanospectroscopy beamline, that brought the energy resolution in the imaging mode down to 100 meV and to 60 meV in the spectroscopy mode, the unique twin fixed-gap adjustable phase undulator that more than doubled the operating energy range of the TwinMic beamline, new state-of-the-art detectors for the Xpress and XAFS beamlines.

The development of the new Elettra 2.0 storage ring continued, with upgrade programs already launched for the SuperESCA, BaDElPh, Spectromicroscopy, XAFS, Nanospectroscopy, TwinMic, and Xpress beamlines, and the construction of a first new beamline for Coherent Diffraction Imaging (CDI). The new 6-bend achromat enhanced lattice (S6BA-E) will decrease the emittance by a factor of 50 relative to the current storage ring, with an increase in brightness of the current insertion devices by a factor of 30 at 1 keV and by a factor of 180 at 10 keV. The coherent component of the radiation will increase by a factor of 60 at 1 keV. The increase in collimation, brightness and coherence afforded by the new Elettra 2.0 source will be exploited to enhance analytical capabilities for spatially inhomogeneous samples and install additional new beamlines for [U+F048][U+F042]-SAXS, [U+F06D]-XRD, [U+F06D]-XAFS and [U+F06D]-XRF. Studies conducted in collaboration with the Department of Energy of the U.S. have shown that it is theoretically possible to install on Elettra 2.0 RF deflectors (crab cavities) that would provide a subset of pulses of single picosecond duration among the conventional pulses and offer users the option of exploiting the picosecond time resolution or the high average brightness. White papers by SLAC and Fermilab proposing normal conducting or superconductive technology, respectively, for the implementation of the crab cavities are currently being assessed by an international panel.

The FERMI FEL-1 and FEL-2 user facilities remain the only EUV and X-ray FELs worldwide exploiting external seeding. The resulting pulse-to-pulse wavelength, linewidth and intensity stability, together with the possibility of performing two-color and four-wave mixing experiments, make the FERMI source currently unique in the international panorama. The six operating beamlines DiProI, EIS-TIMER, EIS-TIMEX, LDM, MagneDyn and TeraFERMI, together with the two table-top complementary laser facilities T-Rex and CITIUS continued operating throughout the COVID-19 pandemic, although some 44% of the approved experimental proposals by international users had to be postponed. New experimental methods have emerged, such as transient grating techniques in the EUV and soft-X-ray range. Exploiting the higher harmonics of FEL-2, wavelengths as short as 1.6 nm were successfully used to excite the L2,3 edges of Fe and Co. Another breakthrough arrived this year, with the synthesis of an attosecond pulse train. Using FERMI, the phase relationship between the pulses could be measured and controlled, allowing “sculpting” of the light to produce an arbitrary wave form. This is a “game changer” in the field of short-wavelength, non-linear optics.

About

Alfonso Franciosi, a national of Italy and of the U.S., is the current Chairman of the Board and CEO of EIlettra Sincrotrone Trieste S.C.p.A. and a Professor of Physics with the University of Trieste. He is responsible for the operation of the 2.4 GeV, third-generation synchrotron radiation source Elettra and of the new free-electron laser source FERMI. He directs a staff of 400 scientists, engineers and support personnel, who conduct in-house research and assist over 2000 international users of synchrotron radiation per year. Such users have at their disposal 38 operating beamlines on the Elettra storage ring and on the FERMI free electron laser and several support laboratories. The publication list of professor Franciosi includes more than 300 articles in refereed international journals on the physics and materials science of semiconductors, semiconductor heterostructures, superlattices, quantum wells, metal/semiconductor contacts, thin film nucleation and growth, lasers and optical modulators, synchrotron radiation spectroscopies and microscopies. Professor Franciosi has been the advisor of more than 40 doctoral and master students in Italy and in the U.S. His former students are now employed by industrial concerns such as Intel, 3M, IBM, Xerox, Cypress Semiconductor Corporation, etc.

Primary author(s) : Dr. FRANCIOSI, Alfonso (Chief Executive Officer Elettra Sincrotrone)

Presenter(s) : Dr. FRANCIOSI, Alfonso (Chief Executive Officer Elettra Sincrotrone)

Session Classification : Plenary Lecture

Contribution ID : **4** Type : **Presentation**

PROTEIN CRYSTALLOGRAPHY IN ACTION VIA X-RAY TECHNIQUES AT THE SYNCHROTRON FACILITIES

Tuesday, 22 June 2021 09:00 (1:00)

Abstract

At the end of the XX Century, most investigations were focused on structural elucidation of large macromolecular complexes for applications in Medicine and Drug´s Design. Recently, techniques like X-ray diffraction, Small Angle X-ray Scattering (SAXS), X-ray Powder Diffraction, Neutron and Electron Diffraction techniques have emerged to obtain the 3D structure of important biological macromolecules for a variety of applications in Structural Biology, Materials Science and Structural Genomics research. Particularly, the X-ray diffraction techniques, which are a hallmark in this search, as these are the most powerful techniques for structure elucidation of biological macromolecules, reaching quasi-atomic resolution in the most favorable cases, and without a priori limitations on the size and complexity of the studied molecules, requires crystals of a high quality. New techniques are emerging like the free electron lasers (FELs) with requirement of micro to nano-sized crystals to solve the 3D structure of very important macromolecular complexes. The XFEL facilities, which generates extremely intense X-ray pulses of tens of femtoseconds duration with nine-to-ten orders of magnitude higher peak brilliance than third-generation synchrotrons tend to get the 3D structure of any macromolecules. Finally, as we have learnt from recent publications cryo-EM with near-atomic resolution for biomolecular structures is one of the most promising techniques to solve the 3D structure of large macromolecular complexes and recently even small molecular weight proteins have been solved.

The aim of this talk will be concentrated on showing the Crystallography in Action, a modern concept to elucidate peculiar biomolecules important in biology or biomedical sciences. The author has sorted out some answers related to basic scientific questions from his laboratory using synchrotron techniques: 1) What is the role of the intramineral proteins into the biomineralization of calcium carbonate? What is the crystallographic role of these biological part and mineral part to understand the evolution of the dinosaurs found in the Northern part of Mexico? Would it be possible to recover ancestral proteins? 2) What is the importance of synchrotron radiation to investigate the 3D structure of biological macromolecules, which are difficult to solve by conventional X-ray in-house diffraction? 3) Polyphenol Oxidase from Vitis vinifera, Cytochrome C from Bovine´s heart and Apo and Holo Human Transferrins: Are these proteins easy to crystallize and be solved by conventional X-ray diffraction or do we need to grow the crystals in situ and to use synchrotron facilities to sort out this structural problem? Can we use non-conventional methods of crystal growth to obtain crystals of different size and appropriate crystal quality to get high resolution structures even for membrane proteins? Finally, the end of this talk will focus on showing how we still lack a unique powerful technique that will help us solve all the structural problems that are arising. Therefore, by crystallography in action, we are looking further into the future in the hope of finding out different ways to solve the 3D structure of proteins that are recalcitrant to crystallize properly, or that are structurally disordered. Based on that, we intend to use the XFEL as the final aim of all these kinds of research projects.

About

Dr. Abel Moreno is a full Professor of Biological and Physical Chemistry at the Institute of Chemistry of the National Autonomous University of Mexico (UNAM) in Mexico City. He has been distinguished as a member of the National System of Researchers of Mexico

(SNI) at level 3 (the highest category of Mexican scientists), a member of the Mexican Academy of Sciences, Mexican Society of Crystallography, Mexican Society of Synchrotron Light, the New York Academy of Sciences, and member of the Mexican and American Chemical Societies. Dr. Abel Moreno has published more than 108 papers in prestigious international journals cited 2300 times having a H-index of 25. He is the author of 15 book chapters and 7 books on his specialties in Biological Crystallogenesis, Crystallochemistry, and Biomineralization processes. Into the Academia he has graduated more than 30 students at all levels from BSC up to the PhDs and postdoctoral fellows. Prof. Moreno was the former President of the International Organization for the Biological Crystallization from September 2010 to September 2012 (IOBCr). Doctor Moreno is an expert in Protein Crystallization, Crystal Growth Methods, Crystallochemistry, Protein Crystallography, Biomineralization Processes and Structural Research using X-ray Diffraction, Scanning/Transmission Electron Microscopy, Atomic Force Microscopy and Synchrotron Radiation Techniques. His work as well as contributions have been applied to Biological Chemistry and Biomedical Sciences.

Primary author(s) : Dr. MORENO, Abel (Institute of Chemistry. UNAM)

Presenter(s) : Dr. MORENO, Abel (Institute of Chemistry. UNAM)

Session Classification : Plenary Lecture

Contribution ID : **5** Type : **Presentation**

XAFS AS A TOOL TO STUDY CHEMICAL STATES AND LOGICAL STRUCTURES

Tuesday, 22 June 2021 10:00 (1:00)

Abstract

X-ray Absorption Fine Structure (XAFS) spectroscopy is one of the most used methods at synchrotron facilities. XAFS is divided into two regions: x-ray absorption near edge structure (XANES) and extended x-ray absorption fine structure (EXAFS). XANES is a region of spectra from just below absorption edges to 3050eV above edges. EXAFS includes higher energy region above XANES usually up to ˜600-800, even up to 1000 eV, and is used to determine local structures around elements of interest. One can obtain bond lengths and coordination numbers, for instance, around elements of interest. Information is obtained element specifically, because energies of absorption edges are element specific. For example, Fe K-edge is about 7112 eV, and Co K-edge 7709 eV. In my talk, fundamental concepts of XAFS are introduced, and several topics on XAFS studies will be shared.

About

Hitoshi Abe was born in Tokyo, Japan in 1980. He initiated surface and ultrathin film magnetism studies in Prof. Toshiaki Ohta's group at the Universityy of Tokyo. He received his master degree in Chemistry from the University of Tokyo in 2005. Under the supervision of Prof. Tetsuya Hasegwa, he received his doctoral degree (Science) from the University of Tokyo in March 2008. He had been a special research fellow of Japan Society for the Promotion of Science from April 2005 to March 2008. In April 2008, he started to work as a research associate at Department of Chemistry, Keio University. His research interests also include surface chemical reactions and development of surface chemistry and magnetism analysis methods with synchrotron x-ray radiation. In April 2010, he moved to Institute of Materials Structure Science, High Energy Accelerator Research Organization as associate professor.

Primary author(s) : Dr. ABE, Hitoshi (Institute of Materials Structure Science. Accelerator Research Organization (KEK))

Presenter(s) : Dr. ABE, Hitoshi (Institute of Materials Structure Science. Accelerator Research Organization (KEK))

Session Classification : Guest Lecture

Contribution ID : **6** Type : **Presentation**

SYNCHROTRON LIGHT FOR THE MICRO-ANALYSIS OF ARTISTIC MATERIALS

Tuesday, 22 June 2021 11:30 (1:00)

Abstract

How did Rembrandt produce his impastos? Why some of the chrome yellows used by van Gogh in the Sunflowers do not show their original colour? Did Egyptian and Roman crafstmen use the same methods to produce opacified glasses? These are typically questions to which chemical analyses can contribute to answer. Indeed, the application of analytical chemistry to decipher the composition and state of conservation of artworks has been intensely increasing over the last decades. Among the many methods available, X-ray microscopy techniques are particularly suitable since they reveal not only the material composition but also the location of the different components. This is very useful to understand a posteriori the artists and craftsmen techniques but also to identify degradation products. Different synchrotron based techniques can be combined (micro X-ray fluorescence, micro X-ray absorption spectroscopy, micro X-ray diffraction) providing various contrasts and allowing to locally tackle the materials via different chemical points of view. In my talk, I will present experiments recently carried out at the European Synchrotron Radiation Facility (ESRF), Grenoble, France. Researchers come from all over the world, bringing tiny samples, to reveal subtle chemical signatures characteristic of certain artistic productions, or, unfortunately, past or on-going alterations. The examples will illustrate the very wide range of artistic materials which can be studied (paintings, ceramics, glasses, manuscripts, photographs, plastics. . .), the different techniques which can be used and the many pieces of information they provide. I will also briefly present the ESRF upgrade phase 2, in particular the new EBS (extremely bright source) and the on-going instrumental developments, explaining how they will contribute to the cultural heritage field.

About

Marine Cotte, researcher at the French National Centre of Scientific Research (CNRS), is currently seconded at the European Synchrotron Radiation Facility (ESRF) in Grenoble, France, where she develops new technologies to examine works of art and archaeological objects. Her research is of enormous value to society because it provides the basis for managing and protecting important examples of cultural heritage. By working with museums, she joins the interests of science to those of society and links cultural heritage to advanced technology. Marine is a pioneering and dedicated researcher who herself took the first steps towards working with Dutch researchers. Receiving the Descartes-Huygens Prize will allow her to go to the Netherlands several times to work with researchers at Delft University of Technology, Eindhoven University of Technology, the Rijksmuseum in Amsterdam and other institutions. She will enter into new alliances with museum conservationists, curators, art historians and technical scientists.

Primary author(s) : Dr. COTTE, Marine (Head of the ID21 Beamline. ESRF)

Presenter(s) : Dr. COTTE, Marine (Head of the ID21 Beamline. ESRF)

Session Classification : Plenary Lecture

Contribution ID : **7** Type : **Presentation**

SHINING SYNCHROTRON LIGHT AT THE NANOSCALE: NANOMATERIALS IN THE BIOSPHERE

Tuesday, 22 June 2021 12:30 (1:00)

Abstract

The ID21 beamline at the European Synchrotron Radiation facility (ESRF) is dedicated to micro X-ray fluorescence (μXRF) and micro X-ray absorption spectroscopy (μXAS) in the tender X-ray range (2-10keV). It has an important scientific activity in the fields of life and environmental sciences, in particular for studying the fate of metals in the environment. This includes, e.g. the study of pollutants, nutrients and innovative drugs, with increasing applications in the field of nanotechnology. Elemental speciation determines the distribution at tissue and cellular level, and ultimately the various mechanisms of action. The chemical form and distribution of elements are also important to environmental risk assessment. ID21 offers a reliable and easy-to-operate passively cooled cryogenic stage, as well as the required auxiliary equipment for sample transport, storage and preparation. Thus, cryo-fixed samples are better preserved under intense X-ray beams and the elemental distributions, chemical states, and sample morphologies are close to the in-vivo state under frozen-hydrated conditions. This presentation will highlight experiments performed at ID21 taking full advantage of these beamline capabilities to investigate the distribution and speciation of engineered nanomaterials in complex biological samples (plant, animal tissues, cells). Finally, the future capabilities expected with the refurbishment of ID21 in the context of ESRF-EBS upgrade will be presented.

About

PhD in Environmental Science and Engineering in 2011 from the University of Texas at El Paso, USA. His research interests focus on the use of synchrotron X-ray fluorescence (XRF) and X-ray Absorption spectroscopy (XAS) at the micro and nano scale to study the distribution and biochemical modifications of trace elements and nanomaterials in biological systems. In 2011, he arrived at ESRF beamline ID21 as post-doctoral researcher. He participated on the development and optimization of cryogenic sample preparation and analysis protocols for XRF and XAS micro-spectroscopy at ID21. He was the responsible scientist of the Infrared branch at ID21 (dismounted in 2017). Since 2013, he is scientist at ID21 (permanent since 2017) where he develops an in-house research program focusing on the characterization of nanomaterials in biological samples and their impact on the environment, particularly on agricultural systems. He is currently the project coordinator of the upgrade program of ID21 that will deliver a new end-station for XRF and XAS nano-analysis with optimized cryogenic environment compatible with biological samples. He has authored and co-authored 90 peer reviewed and 2 book chapters (h-index 26, 2660 citations google scholar). He has co-supervised 2 master thesis, 4 PhD students, and 2 post-doctoral fellows since 2013.

Primary author(s) : Dr. CASTILLO MICHEL, Hiram (X-Ray Microspectroscopy Beamline ID21. ESRF)

Presenter(s) : Dr. CASTILLO MICHEL, Hiram (X-Ray Microspectroscopy Beamline ID21. ESRF)

Session Classification : Guest Lecture

Contribution ID : **8** Type : **Presentation**

SMALL ANGLE X-RAY SCATTERING (SAXS) IN COMBINATION WITH OTHER TECHNIQUES, EXPERIMENTAL AND NON, TO DEAL WITH SOME TOUGH PROTEIN STRUCTURES

Wednesday, 23 June 2021 09:00 (1:00)

Abstract

Small Angle X-ray Scattering (SAXS) is a powerful technique that is used to obtain structural information of both ordered and disordered biological molecules at low resolution. It provides information about the size and shape of proteins and complexes, as well as about structural changes that occur at different experimental conditions [1]. SAXS requires small (milligram) amounts of purified and monodisperse samples. The experiment can be performed rapidly using the dedicated beamlines at synchrotron light sources [2]. Even data analysis, when the quality of the sample is good enough, can be fast, thanks to powerful specialized software [3]. SAXS is a particularly useful technique for the characterization of multidomain proteins [4], which consist of two or more domains connected by linkers determining their flexibility. In a typical SAXS experiment, a collimated monochromatic X-ray beam illuminates a solution of particles, and the intensity of the scattered X-rays is registered by a detector. The recorded scattering pattern is reduced to a radially averaged one-dimensional scattering profile, which results in low structural resolution but can still provide important structural information. In contrast, Macromolecular Crystallography (MX) is an older and mature technique capable of revealing high-resolution details of biological macromolecules when good-sized and well-ordered crystals of such molecules are obtained. Information obtained from different biophysical experiments can be combined to obtain structural insights represented by molecular models. Combination of X-ray crystallography with SAXS data and other techniques including Molecular Dynamic simulations (DM), protein-protein docking, cryo-EM, NMR chemical shift perturbation or FRET and has proven very useful for obtaining detailed models of dynamic protein complexes. Some cases of proteins involved into the mechanism of ribosome biogenesis (Schwachman Diamond Syndrome) [5-6], endoplasmic reticulum quality control (ERQC) machinery [7] and human magnesium transport mediator [8] will be presented.

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About

Dr. Dritan Siliqi is senior scientist at Institute of Crystallography, Italian National Council of Research (IC-CNR and head of Bio-Crystallization Lab. Since 1994, Dr. Siliqi spent a part of his carrier on developing phasing techniques to solve protein structure from X-ray and neutron diffraction data. He is an expert on Small-Angle X-ray Scattering (SAXS) technique applied to biomolecules, and in combination with Wide-Angle Xray Scattering (WAXS) in scanning mode, for the study of biomaterials. He is author of more the 120 papers in international journal. He has been the as coordinator and participant of various and different scientific bilateral agreements with countries such as Mexico, Peru, Brazil, Argentina, UK, Albania, Morocco, and as well of European and National projects. He has also a long experience on experiments at various Xray (MX, SAXS) synchrotron beamlines (ESR, Diamond, DESY, SLS, LNLS) or neutron sources (LANSCE, ISIS). Dr. Siliqi was involved as well as lecturer/tutor at OPEN SESAME HERCULES School for the training of young researchers of the new SESAME synchrotron in Jordan.

Primary author(s) : Dr. SILIQI, Dritan (Institute of Crystallography-CNR)

Presenter(s) : Dr. SILIQI, Dritan (Institute of Crystallography-CNR)

Session Classification : Plenary Lecture

Contribution ID : **9** Type : **Presentation**

ADVENTURES IN "THE LIGHT SOURCELAND"

Wednesday, 23 June 2021 10:00 (1:00)

Abstract

Light Sources are multidisciplinary and interdisciplinary in character, a researchers true "playground". Our adventure starts with forefront research and our a model to develop the next generation in STEM.
The Center for Biomolecular Structure (CBMS), National Synchrotron Light Source II (NSLS II), Brookhaven National Laboratory (BNL), addresses a wide range of environmental and life science questions by operating a suite of experimental facilities opening a wide range of opportunities that allows visiting researchers, partners, and collaborators to succeed in their hypothesis-driven research. In collaboration with the Office of Education (BNL), program "Student Partnerships for Advanced Research and Knowledge" (SPARK) we seek to promote the interdisciplinary and multidisciplinary aspects of science today. The program provides the opportunity for high school students and their educators to become visiting researchers at NSLS II and develop their hypothesis-driven research in partnership with our scientists. This program, now in its fifth year, is an example of the importance of early on collaborations and partnerships between fore-front research facilities and educational institutions.
Acknowledgment: We wish to thank Dr Aleida Perez, for her leadership, SPARK program. We thank the CBMS team, OEP staff and scientific staff on the imaging and spectroscopy beam lines at NSLS II for making the SPARK a success. Our funding agencies, NIH-NIGMS #P30GM133893, DOE-BER #KP1605010, DOE-BES #DE-SC0012704 and BNL-BSA.

About

Vivian Stojanoff works at the U.S. Department of Energy's Brookhaven National Laboratory. There, she uses x-rays at the National Synchrotron Light Source (NSLS) to study how atoms are arranged in protein crystals, because the arrangement affects how proteins function. For example, knowing the way atoms are arranged in the protein insulin has helped medical doctors provide better treatments for diabetes. Stojanoff was raised in Brazil, where she earned her bachelor's and master's degrees in physics and her Ph.D. in crystallography at the University of São Paulo. Before joining the NSLS as a physicist in 2001, Stojanoff held scientific staff positions at the Physics Institute of the University of São Paulo, Brookhaven Lab's Biology Department, and the European Synchrotron Radiation Facility. In addition to her research at Brookhaven, Stojanoff inspires up-and-coming women in STEM fields by heading the Brookhaven Women in Science (BWIS) organization at the Lab. Under Stojanoffs leadership, BWIS hosts seminars and lectures each month, some featuring renowned women scientists from around the world. BWIS also administers two scholarships to women pursuing degrees in STEM-related fields and provides frequent networking opportunities for members to support each other's efforts on the job and encourage each other's successes.

Primary author(s) : Dr. STOJANOFF, Vivian (Brookhaven National Laboratory. National Synchrotron Lightsource)

Presenter(s) : Dr. STOJANOFF, Vivian (Brookhaven National Laboratory. National Synchrotron Lightsource)

Session Classification : Plenary Lecture

Contribution ID : **10** Type : **Presentation**

MACROMOLECULAR CRYSTALLOGRAPHY DATA PROCESSING WITH DIALS

Wednesday, 23 June 2021 11:30 (1:00)

Abstract

The DIALS project provides an open-source toolbox for single crystal diffraction image processing and analysis tasks. DIALS was originally developed as a collaboration between Diamond Light Source, the Lawrence Berkeley National Laboratory and CCP4 to address the needs of advanced light sources, where rapidly-developing technology and experimental methodology have changed the way modern crystallography is performed. The flexible and modular design of the toolbox combines established algorithms alongside novel methods, and provides interfaces at multiple levels of detail. This facilitates a wide scope of use cases, from automated data processing pipelines at synchrotron beamlines, through to user-driven operation of the software using a graphical user interface or a suite of command-line programs. At the lowest level, new software or specialist scripts can be produced by using DIALS as a Python library. Indeed, it is hoped that the open, collaborative nature of the project will inspire the next generation of scientists working on methods development. In this presentation, the main features of the DIALS package will be described, in particular focusing on its use for fast, high quality integration by 3D profile fitting in the context of synchrotron rotation experiments. Examples of some of the novel developments that have come out of the DIALS project will also be given, including algorithms for indexing multiple lattices, improved background determination for weak data collected on pixel array detectors, and clustering methods for multi-crystal data sets. Active areas of current development will be touched upon. These include better modelling for serial snapshot crystallography and adaptations for electron and neutron diffraction experiments.

About

Provides and supports an integrated suite of programs for determination of macromolecular structures by X-ray crystallography; aims to develop cutting edge approaches to experimental determination and analysis of protein structure; as a community based resource, supports the development and integration of novel software into the suite; serves the widest possible research community, embracing academic (not for profit) and for profit research. Offers education and training of scientists in experimental structural biology and encourages the wide dissemination of new ideas, techniques and practice.

Primary author(s) : Dr. WATERMAN, David (STFC Rutherford Appleton Laboratory. Scientific Programmer)

Presenter(s) : Dr. WATERMAN, David (STFC Rutherford Appleton Laboratory. Scientific Programmer)

Session Classification : Guest Lecture

Contribution ID : **11** Type : **Presentation**

SESAME: AN OPPORTUNITY FOR SCIENCE AND GROWTH

Wednesday, 23 June 2021 12:30 (1:00)

Abstract

SESAME (Synchrotron-light for Experimental Science and Applications in the Middle East) is a third-generation 2.5 GeV synchrotron light source in Allan (Jordan) that was officially opened on 16 May 2017. It is the Middle East's first major international research centre and has been hosting users for experiments at its beamlines since July 2018. It is a cooperative venture by scientists and governments of the region set up on the model of CERN (European organization for Nuclear Research) although it has very different scientific aims. It was developed under the auspices of UNESCO as an autonomous intergovernmental organization at the service of its Members. The current Members of SESAME are Cyprus, Egypt, Iran, Israel, Jordan, Pakistan, Palestine, and Turkey. Current Observers are Brazil, Canada, the People's Republic of China, the European Organization for Nuclear Research (CERN), the European Union (EU), France, Germany, Greece, Italy, Japan, Kuwait, Portugal, Russian Federation, Spain, Sweden, Switzerland, the United Kingdom, and the United States of America.

The Phase 1 beamlines have been selected on the basis of input from five scientific workshops and the early Users' Meetings in which several hundred Middle East scientists participated. Three of these beamlines are currently in operation and open to users. They are the XAFS/XRF (X-ray Absorption Fine Structure/X-ray Fluorescence) spectroscopy), IR (Infrared) spectromicroscopy and MS (Materials Science) beamlines. Three more (one for X-ray tomography and two for soft X-ray spectroscopy) are under construction and are expected to come into operation in 2022 and in 2023. The MX (Macromolecular Crystallography) beamline is presently being designed, while the plans for the SAXS/WAXS (Small Angle and Wide Angle X-ray Scattering) are yet to start.

About

Andrea brings with him extensive experience in the science programme of synchrotron light facilities having worked at Elettra-Sincrotrone Trieste S.C.p.A. in Trieste (Italy) since 1996. His recent positions at the Italian Laboratory included Head of the XPRESS beamline for high pressure studies, a position he held until he joined SESAME, Head of Elettra's MCX Powder Diffraction beamline (2008-2015) and Head of the Laboratory's Powder Diffraction beamline (2002-20O08). Since 2008 he has also been in charge of coordination between all the user beamlines and the machine group at Elettra. Andrea also brings long-standing experience in science communication having been a member, since May 2013, of the Communication Task Force of Elettra, and the person responsible for the Elettra content at lightsources.org. Moreover, in April 2019 he was appointed Chair of the RICE (Research Infrastructure Communications and Engagement) working group of the ERF-AISBL (Association of European-Level Research Infrastructures Facilities). Andrea has carried out research in numerous areas and has been an invited teacher in several crystallography and instrumentation schools.

Primary author(s) : Dr. LAUSI, Andrea (Scientific Director, SESAME.)

Presenter(s) : Dr. LAUSI, Andrea (Scientific Director, SESAME.)

Session Classification : Plenary Lecture

Contribution ID : **12** Type : **Presentation**

SYNCHROTRON CRYSTALLOGRAPHY AND THE PHYSICAL PROPERTIES OF FUNCTIONAL POLYCRYSTALS

Thursday, 24 June 2021 09:00 (1:00)

Abstract

Various applications of synchrotron light to the investigation of the structure-properties relationship in polycrystalline functional materials are described. The first part of the presentation is devoted to structural analysis using various experiments with synchrotron light. High resolution diffraction experiments are shown to clarify crystal symmetry, two-dimensional diffraction measurements to characterize the texture of functional polycrystals, and x-ray absorption spectroscopy investigations to characterize short-range order and identify crystalline and amorphous minor compounds. In the second part, the way in which fine structural determinations explain and / or allow to predict tensor physical properties of single- and polycrystals is discussed. Attention is focused on the elasto-electromagnetic properties. The specificity of the single-crystal piezoelectric and magnetoelectric properties is discussed using arguments from group theory. The prediction of textured polycrystals' properties is considered. The adaptation of the Voigt, Reuss and Hill descriptions to the case of the above mentioned properties is presented. The open database "Material Properties Open Database" (MPOD, http://mpod.cimav.edu.mx) is presented and representative cases of the problems described are discussed.

About

Luis E. Fuentes-Cobas obtained his bachelor's, master's, and doctorate in solid state physics from the University of Havana (UH, Cuba). He developed a post-doc on neutronographic texture analysis at the Joint Institute for Nuclear Research Dubna (Russia). The academic interest of Dr. Fuentes-Cobas has been focused on the teaching and research of electromagnetism, the structural analysis of materials by means of synchrotron light and the structure-properties relationship in functional solids. His CIMAV Crystallography Group (mainly graduate students) has solved with synchrotron light the crystal structures of various piezoelectrics and multiferroics, created computer programs for the interpretation via modeling of two-dimensional diffractometric data and contributed novel algorithms for the prediction of the elasto-electro-magnetic properties of textured polycrystals. Dr. Fuentes-Cobas is coordinator of the international project "Material Properties Open Database (MPOD)", associated with the open database http://mpod.cimav.edu.mx, and of the scientific education project "Materials World Modules-México". He is the author or co-author of 150 articles and 7 books, has directed 40 graduate theses. He has received scientific awards in Russia and in Cuba. In 2012 he received the Chihuahua State Prize for Science, Technology and Innovation.

Primary author(s) : Dr. FUENTES COBAS, Luis Edmundo (Materials Physics. Advanced Materials Research Center); Dr. MONTERO CABRERA, María Elena (Materials Physics. Advanced Materials Research Center)

Presenter(s) : Dr. FUENTES COBAS, Luis Edmundo (Materials Physics. Advanced Materials Research Center); Dr. MONTERO CABRERA, María Elena (Materials Physics. Advanced Materials Research Center)

Session Classification : Plenary Lecture

Contribution ID : **13** Type : **Presentation**

CHARACTERIZATION OF CATHODE MATERIALS USING X-RAY ABSORPTION SPECTROSCOPY AND X-RAY FLUORESCENCE AT ELETTRA-SINCROTRONE TRIESTE

Thursday, 24 June 2021 10:00 (1:00)

Abstract

Accelerating the transitions to low carbon economy calls for rigorous and relevant research in various disciplines including, among others, energy storage and conversion which are essential to face increasing sustainability challenges in tackling global warming and energy security. Indeed, the renewable energies request the use of efficient electric energy storage systems to maximize the profit and benefit of all the energy generated. In this context, much effort is being made to design safe, lightweight, small and environmentally friendly batteries, with a high-energy density and long run and lifetimes, sometimes in an all-in-one solution. I will present the activity of the XAFS and XRF beamlines at Elettra- Sincrotrone Trieste in the field of energy storage materials highlighting the role of analytical tools such as x-ray absorption and x-ray fluorescence for the characterization of the different parts of an electrochemical cell and in particular the cathode materials. The studies performed at the XAFS beamlines are in operando conditions, i.e. the cathode are investigated during the actual operation of the battery. In these studies x-ray absorption spectroscopy provides information on the electronic and local structure of the electrochemically active elements at different points of the charge/discharge cycle, clarifying the role of the metallic ions that constitute the cathode materials during the electrochemical reaction. At the XRF beamline instead we have used x-ray fluorescence microscopy to visualize spatial heterogeneities of the active material within the cathode to be possibly correlated with the capacity fading over time after multiple operating cycles. The examples shown concerns both Li-ion and post-Li-ion batteries such as Li-S ans Na-ion batteries and highlight the role and complementarity of advanced analytical tools based of synchrotron radiation.

About

Dr Giuliana Aquilanti is head of beamlines XAFS and XRF at Italian synchrotron in Trieste (Elettra). She received her PhD in Physics at the University Joseph Fourier (Grenoble, France). The research carried out over the last 20 years concerns the development and application of x-ray techniques (mainly x-ray absorption spectroscopy) for the study of matter and was carried out at the European Synchrotron in Grenoble (ESRF) and at Elettra. Her research activity is devoted to two main themes: (a) structural characterization of advanced materials for energy storage, and (b) structural characterization of matter under extreme pressure and temperature conditions. She is coordinating the scientific activity of the XAFS and XRF beamlines staff, as well as supervising fellows within different programs of ICTP, IAEA and IUCr. She was involved in different research projects funded by EU, IAEA and CERIC-ERIC. She is member and of the XAFS commission of the IUCr and part of the peer review committee of synchrotron Soleil. She is co-author of more than 170 articles.

Primary author(s) : Dr. AQUILANTI, Giuliana (Head of XRF Beamlines. ELETTRA-Sincrotrone Trieste)

Presenter(s) : Dr. AQUILANTI, Giuliana (Head of XRF Beamlines. ELETTRA-Sincrotrone Trieste)

Session Classification : Guest Lecture

Contribution ID : **14** Type : **Presentation**

PRESENT AND FUTURE OF THE ALBA SYNCHROTRON IN SPAIN

Thursday, 24 June 2021 11:30 (1:00)

Abstract

Over the past decade, the ALBA Synchrotron, the Spanish 3rd generation light source, has become an important pillar of the Spanish and European Research Area, providing research capabilities and a wide range of state-of-the-art instrumentation to a community of more than 6000 academic and industrial users. With its ten operating beamlines, while building three more, it is an essential tool for addressing the most urgent challenges of the society. ALBA dedicated industrial program impacts directly the economic growth offering new development opportunities and ultimately windows of innovation for a variety of companies. ALBA plays today an important role in science tutoring and training, preparing young scientist and engineers for their future career, and is a tool for education of the general public. ALBA is prepared to leap to the 4th generation, boosting its impact on the user community and on the industrial use of the instrumentation, and reinforcing its educational vocation and training capacity. ALBA II, whose project has just started, will combine the substitution of part of the accelerator with the construction of new fully-optimized beamlines, and with the refurbishment of part of its instrumentation, to be fully operative in the '30s.

About

La Dra. Caterina Biscari es una física, directora del Sincrotrón ALBA. Licenciada en Física por la Universidad Complutense de Madrid y Doctora en Física por la Universidad degli Studi di Napoli, ha desarrollado su carrera científica en el ámbito de los aceleradores de partículas en diversos laboratorios del mundo, como la Organización Europea para la Investigación Nuclear (CERN), el Laboratorio Nazionale de Frascati del INEN y el Centro Nacional de Hadronterapia Oncológica de Pavia, contribuyendo al desarrollo de aceleradores para investigación fundamental, investigación aplicada y aplicaciones médicas. Es EPS Fellow por sus contribuciones claves en el diseño, la construcción y la puesta en marcha de aceleradores. Desde 2012 es Directora del Laboratorio de Luz de Sincrotrón ALBA. Miembro de comités asesores de proyectos en diversos países, entre otros el comité asesor de los aceleradores del CERN, de la Fuente Europea de Neutrones ESS, de la fuente de fotones Europea XFEL. En 2012 recibió la condecoración de Oficial de la Estrela de Italia.

Primary author(s) : Dr. BISCARI, Caterina (Director of ALBA Synchrotron)

Presenter(s) : Dr. BISCARI, Caterina (Director of ALBA Synchrotron)

Session Classification : Plenary Lecture

Contribution ID : **15** Type : **Presentation**

TRENDS ON THE MICROSTRUCTURE AND PATHOLOGY OF CONCRETE RESEARCH WITH SYNCHROTRON RADIATION

Thursday, 24 June 2021 12:30 (1:00)

Abstract

At present, the construction industry has a big challenge in favor of the environment, having among other objectives, reduce CO2 emissions, construction waste, and the use of natural aggregates. Therefore, to improve the durability and longevity of concrete, sustainably, conventional techniques are often used to analyze and characterize cementitious materials, aggregates, additives and admixtures, to explore the morphology, composition, and crystalline structure of the materials, and the composites used in construction. However, in the last decade, techniques based on synchrotron radiation (SR) are elucidating the interaction of such materials in more detail, thanks to their high spectral and spatial resolution. Techniques, such as Scanning Transmission X-ray Microscopy (STXM), microtomography (uCT), high-pressure X-ray diffraction (XRD), among others; are making it possible to investigate deeper and efficiently the microstructure of cementitious mixtures, the phenomenon of hydration, crystallization, polymerization. Besides, it is becoming easier to visualize and analyze the generation and distribution of pores; the interaction of additives, and admixtures in the cementitious matrix. And lately, the effect of solid waste (crushed glass and concrete) used as aggregates. On the other hand, pathologies due to aggregate reactivity, chloride, sulfate, CO2, and other aggressive elements to the construction components, can be studies as well. Overall, the studies performed with SR techniques are contributing greatly to the knowledge of deterioration processes and the pathologies in mortars, concrete, and edifications, and are helping to improve the durability and longevity of buildings sustainably.

About

El Dr. Daniel Hernández Cruz es Profesor Tiempo Completo de la Facultad de Ingeniería de la Universidad Autónoma de Chiapas. Es lngeniero Electrónico por Instituto Tecnológico de Tuxtla (ITTG). Obtuvo el grado Maestro en Ciencias con la Especialidad en Óptica por el Instituto Nacional de Astrofísica, Óptica y Electrónica (INAOE). Es Doctor en Fisica por la Université Laval, de Quebec, Canadá, en el año 2004. Del año 2004 al 2007 realizó trabajos de investigación como Posdoctorante para McMaster University en Ontario, Canadá, estando de base en el Advanced Light Source del Lawrence Berkeley National Laboratory, en California, Estados Unidos. Entre los años 2007 y 2008 realizó, como posdoctorante, trabajos de investigación con el grupo de Nanociencias y Nanotecnología en el Instituto Potosino de Investigación Científica y Tecnológica (IPICYT). Del 2008 al 2009 se incorporó a la Facultad de Ingeniería de la UNACH para realizar investigaciones bajo el programa de retención de CONACYT. Entre el 2012 y 2013 realizó una estancia de investigación como profesor invitado del Prof. Paulo Monteiro, del Departamento de Ing. Civil y Ambiental de la Universidad de California en Berkeley, EEUU, utilizando técnicas basadas en Luz de Radiación Sincrotrón, para el estudio de materiales cementosos.

Primary author(s) : Dr. HERNÁNDEZ CRUZ, Daniel (Faculty of Engineering. Autonomous University of Chiapas)

Presenter(s) : Dr. HERNÁNDEZ CRUZ, Daniel (Faculty of Engineering. Autonomous University of Chiapas)

Session Classification : Guest Lecture

Contribution ID : **16** Type : **Presentation**

SYNCHROTRON LIGHT APPLICATIONS IN LIFE SCIENCES

Friday, 25 June 2021 09:00 (1:00)

Abstract

Complex questions such as understanding mechanisms of metal homeostasis in biological systems can be addressed through use of hybrid methods which enable studies at different length and time scales. These approaches may involve complementary use of techniques like macromolecular crystallography which yields the structure at atomic resolution together. with spectroscopic imaging which may provide spatial information. Similarly, information from time resolved solution X-ray scattering experiments may be combined with cryoEM to follow conformational changes during protein-protein or protein-ligand interactions. Advanced instrumentation at synchrotron radiation sources provide a wide spectrum tools for structural studies of biological systems at different levels. Specifically, macromolecular crystallography, small angle X-ray solution scattering (SAXS), X-ray absorption and fluorescence spectroscopy (XAS), and imaging are enabling studies of structure-function relationships at different resolutions from atomic to cellular scale. In this talk results of experiments with two metal binding proteins; a Cd-binding metallothionein isolated from durum wheat (dMT) and the periplasmic ferric binding protein from H. influenzae (FbpA) will be presented. For dMT, combined results from SAXS, circular dichroism, absorption spectroscopy and in situ dMT expression studies show that the apo protein has a flexible extended structure which stably folds in the presence of metals and that the folded and unfolded conformations are sensitive to environmental pH conditions. For FbpA, differences in conformation between apo and holo forms are shown together with differences with the allosteric mutant D52A. It is also shown that, despite its stable secondary structure the apo protein enough flexibility to accommodate different conformations in solution. These results will be discussed in the context of the current models for metal binding mechanisms for both proteins. Moreover, possible role of dMT in Cd toxicity in humans and how structural features of FbpA may be generalized to other periplasmic transport proteins will be presented.

About

Dr. Zehra Sayers is a molecular biophysicist researching mainly on synchrotron X-ray structure analysis of biological macromolecules. She holds a BSc in Physics (Bogazici University, Istanbul) and a PhD in Biophysics (University of London). She was a post-doc in the UK and Sweden and was a staff scientist at European Molecular Biology Laboratory (EMBL) Hamburg Outstation (1986-1998) before joining Sabanci University in Istanbul as a founding faculty member. Here she was the Director of Foundation Development Program (2010-2019) and served as the interim President in 2018. Currently she is on a sabbatical at the EMBL Outstation in Hamburg. Dr. Sayers has been the Chair of the Scientific Advisory Committee of the international synchrotron radiation facilityy project SESAME (Synchrotron-light for Experimental Science and Applications in the Middle East) from its early stages until 2018. Her contributions to the realization of this project have been internationally recognized with the Rammal Award in 2017 and AAAS Science Diplomacy Award in 2019. She is also an honorary member of the Science Academy of Turkey.

Primary author(s) : Dr. SAYERS, Zehra (Faculty of Engineering and Natural Sciences. Sabanci University)

Presenter(s) : Dr. SAYERS, Zehra (Faculty of Engineering and Natural Sciences. Sabanci University)

Session Classification : Plenary Lecture

Contribution ID : **17** Type : **Presentation**

ION BEAMS AND SYNCHROTRON LIGHT IN PERSPECTIVE

Friday, 25 June 2021 10:00 (1:00)

Abstract

This work is devoted to reflecting on the very different features and dynamics of ion beam and synchrotron facilities and user communities. Whereas both suites of techniques are highly interdisciplinary and offer good science opportunities to similar fields of science, traditionally the two communities have lived in separate worlds, with scarce knowledge of one another and very limited collaboration. Many different techniques have been developed based on synchrotron light during the last decades. If one adopts a very global and non-exhaustive view, some of the main ones may be grouped and summarized as follows: diffraction, photon spectroscopies, electron photoemission spectroscopies and imaging/tomography. The features of each group of techniques may be found elsewhere. These techniques are based on large facilities, with wide user communities, many in-situ possibilities and time-resolved capabilities. Ion beams, again with a broad and non-exhaustive view, may be classified as follows: analysis based on nuclear interations, ion in/ion out, analysis based on atomic/nuclear interaction (ion in/photon out), channeling configuration, modification. The features of each technique may also be found elsewhere. Facilities tend to be medium/small, with a smaller user community, limited in-situ capabilities and rare time-resolved setups. In summary, synchrotron techniques provide extremely rich and diverse tools to understand matter at the nano and mesoscale. This implies a large investment effort and the size of the facilities makes them, as a side-effect, very powerful science hubs, beyond the base contribution of the techniques offered. Ion-based techniques are an excellent complement to synchrotron techniques when depth profiling or trace element detection (possibly with 2D resolution) plays a relevant role. In addition ions may be used to modify materials in unique ways and to understand how these damage processes, crucial in areas such as fusion energy devices, take places and may be managed or mitigated. Ion facilities, being small or medium size, provide a very natural scientific landscape complement to larger synchrotrons in a country. ALBA and CMAM are respectively synchrotron and ion beam facilities located in Spain. They were both built during the 2000 decade, CMAM starting a few years before ALBA. Their relative size may be exemplified by the initial investment (at the level of 200 ME for ALBA and 10 ME for CMAM. Further details may be found in [1, 2] for ALBA and [3, 4] for CMAM. Some examples in which ion beams and synchrotron light may be used in a complementary way are given below. XANES, XRD (synchrotron) and RBS (ions) were used in a complementary way to understand the better the preparation process of Ti oxide films [5]. Here XANES was used to look at the valence states of Cr or Ti averaging along the sample depth, whereas RBS was used to verify the Cr-O or Ti-O stoichiometry as a function of depth. XRD was used in both cases to check crystallinity. PIXE (ions) and XRD (synchrotron) were used to characterize samples which emulate the historical features of Co and As based pigments for ceramic archaeological pieces in [6]. In situ temperature cycling of the samples while doing XRD characterization was used to emulate the ancient manufacturing processes and shed light on the composition differences observed in objects from different periods of the 15th-16th century. An ongoing collaboration between CMAM and ALBA is exploring the possibility of manufacturing X-ray gratings by using ion beam lithography [7]. A particularly challenging material, synthetic diamond, is being used as a possible future option for ultra-high heat load applications in X-ray science. Synchrotron and ion beam facilities and user communities are very different and have historically held very limited collaboration. However the techniques are clearly complementary in a number of ways. This paper aims at illustrating and exemplifying such possible collaborations. One may expect that progress in both synchrotron and ion beam techniques may unlock in the future some scientific opportunities which are today out of reach.

References: [1] G. García, S. Ferrer, The Spanish light source ALBA, Synchrotron Radiation News, 27:1, 30-33 (2013). [2] www.cells.es [3] A. Redondo-Cubero, M. J. G. Borge, N. Gordillo, P. C. Gutiérrez, J. Olivares, R. Pérez-Casero and M. D. Ynsa, The European Physical Journal Plus, pp. 136-175, 2021. [4] www.cmam.uam.es [5] R. Gago et al., Structural impact of chromium incorporation in as-grown and flash-lamp-annealed sputter deposited titanium oxide films, Journal of Alloys and Compounds, 2017, 729, 438-445. [6] J. Molera, A. Climent-Font, G. García, T. Pradell, O. Vallcorba, A. Zucchiatti, Experimental study of historical processing of cobalt arsenide ore for colouring glazes (15-16th century Europe), J. of Archaeological Science: reports 36 (2021) 102797. [7] G. García, M. Díaz-Híjar, V. Tormo-Márquez, I. Preda, O. Peña-Rodríguez, J. Olivares, Structural damage on single-crystal diamond by swift heavy ion irradiation, Diamond and related Materials 58 (2015) 226-229.

About

Gastón García López, director del Centro de Microanálisis de Materiales (CMAM), es licenciado en Ciencias Físicas y en Matemáticas por la UAM y diplomado en Derecho por la Universidad de Valladolid. En el año 2000 se doctoró en Física con la calificación de sobresaliente cum laude. Durante los últimos 13 años ha estado ligado al sincrotrón ALBA (Barcelona), ocupando el cargo de subdirector desde 2013 hasta 2019, periodo en el que fue responsable de proyectos estratégicos. De 2000 a 2006 estuvo ligado al CMAM de la UAM, donde fue coordinador del equipo técnico y vicedirector. Con una amplia experiencia en gestión de infraestructuras de investigación, dirección y coordinación de equipos multidisciplinares y planificación estratégica, Gastón García representa a España como asesor en el Consejo del ESRF (European Synchrotron Radiation Facility) y es presidente del comité de coordinación de LEAPS, red que une a todos los sincrotrones y láseres de electrones libres europeos. Inició su carrera investigadora en el campo de Fisica de Altas Energías, para dedicarse posteriormente a la Ciencia de materiales aplicando técnicas basadas en aceleradores de partículas, con especial énfasis en el daño de materiales inducido por irradiación. Durante los últimos años ha realizado numerosas actividades de divulgación científica.

Primary author(s) : Dr. GARCÍA LÓPEZ, Gastón (Director Centro de Micro-Análisis de Materiales. Universidad Autónoma de Madrid)

Presenter(s) : Dr. GARCÍA LÓPEZ, Gastón (Director Centro de Micro-Análisis de Materiales. Universidad Autónoma de Madrid)

Session Classification : Guest Lecture

Contribution ID : **18** Type : **Presentation**

SYNCHROTRON LIGHT APPLICATIONS IN ARCHAEOLOGY: HEAVY METALS AND HUMAN HEALTH IN THE PAST.

Friday, 25 June 2021 11:30 (1:00)

Abstract

Health is a critical factor for individuals, societies, and economies to thrive. Human heavy metal exposure is topical today, and has affected humanity since the first exploitation of metals, at the core of our civilization. This presentation highlights how synchrotron light, and X-ray Fluorescence (SR-XRF) and X-ray absorption fine structure (XAFS) in particular, can be used to explore not only the presence, but crucially in the context of human health, the speciation of heavy metals in ancient human tissues, including bone, dental tissues, hair and skin. Metals such as lead (Pb), arsenic (As), and copper (Cu), were mined, manufactured, and used at ancient archaeological sites, enabling technological advances. Cultural aesthetics led to the use of heavy metals in pigments decorating artefacts, and in cosmetics for enhancing personal appearance. In my first case study, the ID21 scanning X-ray microscope optimized for 2D µXRF (elemental maps) was used at the ESRF (European Synchrotron Radiation Facility) to obtain detailed elemental maps, including Cu, in ancient human hair sections. Only a handful of studies using synchrotron radiation enabled approaches to ancient human hair have been undertaken to date, few studies explore metal element distribution within ancient hair, and none Cu in particular. Key archaeological questions, such as effects of intensive metal and craft work on human health, can be investigated using synchrotron radiation micro X-Ray Fluorescence (SR-µXRF) in exploring biogenic versus diagenetic/environmental uptake of metals, and copper in particular, in ancient human hair. Through the second case study within this talk I showcase the use of extended X-ray absorption fine structure (EXAFS) to explore heavy metal speciation (Pb) in ancient human tissues in the context of exploring past human health in ancient Iran, using the SESAME (Synchrotron-light for Experimental Science and Applications in the Middle East) XAFS/XRF beamline. Metals allowed humanity to become what it is today, but not without a cost. Synchrotron light enables us to explore human health in the deep past, as well as in the present.

About

Kirsi received her PhD from University of Cambridge (Trinity College) in 2004, with focus on human bioarchaeology. Prior to joining the Cyprus Institute (Cyl) and its Science and Technology in Archaeology and Culture Research Center (STARC) in 2008, Kirsi was the Director of the Wolfson Bioarchaeology Laboratory and tenured Faculty at Newcastle University. At Cyl she served as the Chair of the Faculty Council of the Science and Technology in Archaeology and Culture Research Center. She was the Scientific Coordinator of the EU FP7 project STACHEM (Science and Technology for Archaeology and Cultural Heritage in the Eastern Mediterranean). Kirsi's current research focuses on synchrotron radiation enabled bioarchaeology, as well as other scientific and technological means to approach key questions about the human past through archaeological human tissues, ranging from bone and teeth to hair and skin remains. She currently leads analyses of human remains from the wider Eastern Mediterranean and Middle East (EMME) region and beyond, including Cyprus, Iraq, Syria, Turkey, Iran, and Egypt. Her particular research interests include heavy metal exposure in the past through focus on microstructures of ancient human tissues, using synchrotron radiation techniques. Kirsi currently supervises

five PhD students, engaging them in regular beamtimes at synchrotron radiation facilities at ESRF, SESAME, and PSI (Swiss Light Source). Kirsi led the first official user group at the newly opened SESAME synchrotron, including two of her PhD students.

Primary author(s) : Dr. LORENTZ, Kirsi (The Cyprus Institute)

Presenter(s) : Dr. LORENTZ, Kirsi (The Cyprus Institute)

Session Classification : Guest Lecture

Contribution ID : **19** Type : **Presentation**

ENTENDIENDO LA REGULACIÓN ENZIMÁTICA Y LA EVOLUCIÓN DE TRISAFOSFATO ISOMERASAS DE PLANTAS

Friday, 25 June 2021 12:30 (1:00)

Abstract

Las plantas generan energía mediante el ciclo de Benson-Calvin y consumen energía durante la glucólisis y la fosforilación oxidativa. Las rutas de producción y consumo de energía ocupan una serie de enzimas ancestrales y las reacciones enzimáticas se llevan a cabo tanto en el cloroplasto como en el citosol, bajo condiciones de estrés oxidativo muy distintas. El genoma nuclear de las plantas terrestres codifica para dos versiones de una de estas enzimas, la triosafosfato isomerasa (TPI), un producto génico se localiza en el citoplasma y el otro se importa al cloroplasto. Las TPI citoplásmica (cTPI) y de cloroplasto TPI (pdTPI) se ensamblan como dímeros (β-α)8 con alta homología estructural. cTPI y pdTPI albergan dos y uno grupos tiol accesibles por monómero, respectivamente. Por estudios estructurales encontramos que ambas TPI son reguladas por el ambiente redox por la derivatización de cisteínas específicas. Dado que las TPI han evolucionado por duplicación de genes, la mayor resistencia de pdTPI a los agentes redox puede ser una consecuencia adaptativa al entorno redox en el cloroplasto.

En plantas, una de estas enzimas, la triosafosfato isomerasa (TPI) ancestral de cianobacteria fue remplazada por una versión duplicada de la TPI citosólica. Esta isoforma adquirió una señal de exportación a cloroplasto en donde participa en el ciclo de Calvin-Benson. Para tener un mejor entendimiento acerca del reemplazo estudiamos la TPI de la bacteria fotosintética Synechocystis (SyTPI) en comparación con las TPI de citosol y de cloroplasto de Arabidopsis thaliana. Proponemos que la SyTPIf ue remplazada por una TPI eucarionte debido a que la versión duplicada contenía cisteínas redox-sensitivas que pueden ser objeto de modificaciones postraduccionales, requeridas para la modulación de la actividad enzimática Nuestros estudios dan nos permiten entender como se reorienta el metabolismo del carbón hacia la ruta de las pentosas fosfato para disminuir el estrés oxidativo por medio de modificaciones postraduccionales.

About

Ingeniero bioquímico del ITESM-Campus Guaymas y doctor en ciencias por el Centro de ciencias médicas de la Universidad de Texas-San Antonio, auspiciado por una beca Fulbright-Carcía Robles. Estudios postdoctorales en Harvard Medical School becado por la fundación Pew. Líder del grupo de Bioquímica Estructural del Langebio-Cinvestav. Ha recibido honores como la beca de la fundación Howard Hughes, alumno distinguido de la Universidad de Texas y el nombrarmiento de investigador nivel 3 del Sistema Nacional de Investigadores. Su investigación se fundamenta en la premisa que una estructura vale más que mil palabras. Este paradigma ha sido utilizado en su laboratorio para entender como funcionan los sistemas de replicación mitocondrial en plantas, y diversas enzimas como triosafosfato isomeras, DNA polimerasas y DNA glicosilasas y especialmente para modificar proteinas de manera racional. Cuenta con más de 70 artículos en Pubmed y su ha formado a 12 estudiantes de doctorado y 20 de maestría.

Primary author(s) : Dr. BRIEBA DE CASTRO, Luis Gabriel (Laboratorio Nacional de Genómica. CINVESTAV-Irapuato); Dr. CASTRO, Eduardo (Langebio-Cinvestav); Dr. CASTILLO, Margarita (Langebio-Cinvestav); Dr. JIMÉNEZ, Pedro (Langebio-Cinvestav)

Presenter(s) : Dr. BRIEBA DE CASTRO, Luis Gabriel (Laboratorio Nacional de Genómica. CINVESTAV-Irapuato)

Session Classification : Guest Lecture

Contribution ID : **20** Type : **Presentation**

HIGHLIGHTS OF THE MEXICAN SYNCHROTRON DESIGN

Friday, 25 June 2021 14:30 (1:00)

Abstract

In the design of a synchrotron light source, it is required to put together many important pieces. It is important how magnets are chosen in the right order to guarantee that electrons are turning around the central orbit for long periods of time. Different models are being proposed to upgrade synchrotrons. This presentation will address some ideas developed during the last synchrotron upgrades. Some of these upgrades are the 9BA concept in ALS-U, the hybrid model in EBS-ESRF and the use of anti-bends in SLS-2. They have been considered as possible models for the Mexican synchrotron design. A more thorough study should give insight on the motion of electrons affected by nonlinear dynamic, that comes into play once the chromaticity is corrected. Some codes help to achieve this task, but they present some problems. In reference to minimizing the nonlinear dynamic effects in phase space, a partially elaborated technique is described in this presentation which we think will be useful to increase the dynamic aperture. The method treats the non-linear dynamic of the particles in the synchrotron, by optimizing the parameters of the multipoles that generate such complex behavior. All this is linked to a process of approximating the non-linear problem to the corresponding linear problem by using quasi-invariants.

About

Hizo su doctorado en física matemítica en la UNAM. Posteriormente hizo un posdoctorado en Brookhaven National Laboratory donde tuvo la oportunidad de trabajar en física de aceleradores en el AGS y en el proyecto del Relativistic Heavy lon Collider. Regresó a la Universidad de Guanajuato para participar en la creación de su Instituto de Fisica y en el programa de posgrado correspondiente. Ya en el ICF, se unió en 2007 al grupo nacional que proponía la creación de una fuente de luz sincrotrón en México y desde entonces ha estado ligado a este proyecto participando principalmente en su diseño. Ha colaborado con grupos de biofísica y de física atómica del ICF en el desarrolo de un compuesto farmacológico derivado de la anfotericina B y en modelos de propiedades de membranas lipídicas, así como en experimentos de espectroscopía atómica en líneas de radiación sincrotrón.

Primary author(s) : Dr. ANTILLÓN DÍAZ, Armando (Instituto de Ciencias Físicas. UNAM)

Presenter(s) : Dr. ANTILLÓN DÍAZ, Armando (Instituto de Ciencias Físicas. UNAM)

Session Classification : Guest Lecture

Contribution ID : **21** Type : **Presentation**

SYNCHROTRON AND NEUTRON DIFFRACTION FOR THE STUDY OF STRUCTURAL AND MAGNETIC FEATURES OF MULTIFERROIC

Saturday, 26 June 2021 09:00 (1:00)

Abstract

In hard condensed-matter-physics, there are hot topics that have been developed during the last twenty years: multiferroic materials, low dimensional magnetism, topological insulators, skyrmions, etc. In order to understand the microscopic physical behaviour of this kind of materials, the precise knowledge of the crystal and magnetic structure as a function of temperature or external fields is of paramount importance. For that, single crystal and powder diffraction are necessary. The availability of synchrotron and neutron sources has made possible to increase the precision of structural and magnetic data using powder diffraction. The development of the Rietveld method to refine crystal and magnetic structures was possible because the peak shape of powder diffraction lines, in neutron diffractometers, was nearly Gaussian and this was simple enough to be treated by computers of 50 years ago. Nowadays, the method has been largely improved incorporating new methods of calculating structure factors in terms of symmetry modes or modulation functions. Moreover, more complex peak shapes can be treated easily and the Rietveld method is routinely applied to the treatment of synchrotron and neutron powder diffraction. Concerning magnetic structures, neutron powder diffraction is dominating the scene. Synchrotron X-rays interact with atomic magnetic moments providing X-ray magnetic scattering, however the signal is very weak and single crystals are needed. In this lecture, I will present a comparison of the different characteristics of neutron and X-ray synchrotron radiation for the study of the crystal and magnetic structures of crystalline solid presenting interesting physical properties. I will select few examples to illustrate the advantages and drawbacks of both neutrons and synchrotron X-rays in the study of multiferroic materials and low dimensional magneto-structural phase transitions.

About

Juan Rodriguez-Carvajal (JCR) has been involved in large scale projects for developing new neutron sources, in particular the European Spallation Source (ESS). He was the Coordinator for the Structural Science and Solid State Chemistry group of the Scientific Case of the ESS project (1995-1996); he was member of the Instrumentation Task Group of the ESS (2000-2002) and member of Scientific Advisory Committee of the ESS (2009-2012). JRC has participated in many committees and selection panels for research projects in large scale facilities, in particular at ISIS (U.K.), PSI (Switzerland) and SNS (USA). JRC has, and has had, also a strong activity in training young researchers through many courses on diffraction and crystallography organized by universities and research institutions in many places of the world. During the major part of his career JRC has been interested in the following fields: 1. Data analysis and software development in Crystallography and Diffraction Physics. 2. Theoretical analysis of magnetic Structures. Frustration and low dimensional magnetism. 3. Physics of Transition Metal-Rare Earth and Superconducting oxides and intermetallics.

Primary author(s) : Dr. RODRÍGUEZ CARVAJAL, Juan (Institut Laue-Langevin)

Presenter(s) : Dr. RODRÍGUEZ CARVAJAL, Juan (Institut Laue-Langevin)

Session Classification : Plenary Lecture

Contribution ID : **22** Type : **Presentation**

SOME OF THE FEATURES THAT MAKE RESONANT INELASTIC X-RAY SCATTERING (RIXS) A POWERFUL TOOL TO STUDY THE ELECTRONIC STRUCTURE OF COMPLEX MATERIALS

Saturday, 26 June 2021 10:00 (1:00)

Abstract

RIXS is a photon-in-photon-out technique with unique characteristics that make it an ideal tool to study the electronic structure of compounds. It simultaneously probes the occupied and unoccupied electronic states, providing a detailed picture of projected density of states. RIXS is also sensitive to the oxidation state of the atom being probed, and also to the localization of the excited electron. In this talk examples of the use of these capabilities in the study of the electronic properties of TM perovskites that are particularly useful battery electrodes or solar cells. It will also be discussed how the excited electron localization gives information about fast decay processes in orthovanadates. Possible new directions for RIXS research that take advantage of the advances in resolution (time, space and energy) will also be presented.

About

El Dr. José I. Jiménez Mier y Terán estudió la licenciatura en física en la Facultad de Ciencias de la UNAM. Obtuvo la maestría y el doctorado en el Departamento de Física de la Universidad de Yale. Realizó una estancia posdoctoral en el Oak Ridge National Laboratory. Es investigador del ICN en la UNAM desde 1987. También desde 1987 ha impartido clases en el Departamento de Física de la Facultad de Ciencias de la UNAM. Es Investigador Nacional nivel III. Ha impartido más de 60 cursos de licenciatura y posgrado, la mayoría en la UNAM, pero también en la UAM Iztapalapa y en el Departamento de Física de la Universidad de Tulane. Ha dirigido tres tesis de doctorado, cuatro más de maestría y nueve de licenciatura. Ha sido investigador invitado en el National Bureau of Standards en Gaithersburg, en la Universidad Central de Florida, en el Synchrotron Radiation Center en Wisconsin, en el Advanced Light Source en Berkeley y en los departamentos de física de las Universidades de Tulane y Estatal de New York en Stony Brook. Tiene 52 artículos de investigación en revistas, 17 trabajos publicados en memorias de congreso, un capítulo en libro de investigación, dos artículos en revistas de enseñanza, tres reportes internos y 31 artículos de divulgación. Sus trabajos de investigación han recibido unas 760 citas. También cuenta con notas completas (350 páginas) del curso de Física Atómica y Materia Condensada que imparte regularmente en la Facultad de Ciencias de la UNAM

Primary author(s) : Dr. JIMÉNEZ MIER Y TERÁN, José Ignacio (Instituto de Ciencias Nucleares. UNAM)

Presenter(s) : Dr. JIMÉNEZ MIER Y TERÁN, José Ignacio (Instituto de Ciencias Nucleares. UNAM)

Session Classification : Guest Lecture

Contribution ID : **23** Type : **Presentation**

ESTUDIOS DE CRISTALOGRAFÍA EN SINCROTRÓN: UNA FUENTE DE MARAVILLAS

Saturday, 26 June 2021 11:30 (1:00)

Abstract

This talk will present some of the studies caried out using single crystal photocrystallography. Therefore, an introduction to this technique will be presented and the characteristics of synchrotron facilities that allow these studies to be carried out as well as some of the first studies reported in the literature of the use of photocrystallography. This taljkwill focus mainly on the studies carried out of the photochemical activation of coordination compounds which leads to the formation of linkage isomers. Since the particular technique for each case depends on the lifetime of the excited species; different possibilities will be presented. The main objective of these studies has been the structural characterization of meta-stable complexes formed by the molecules upon radiation at a given wavelength. The experimental method used will be described. A brief discussion on the characteristics of the complexes necessary for these studies will also be presented.

About

B. Sc. In chemistry and M. Sc. In inorganic chemistry; both from the Universidad Nacional Autónoma de México. Ph. D. in Chemistry from Cambridge University in the United Kingdom. Researcher at the Chemistry Instituteca, UNAM for 8 years. Since 1991, researcher at the Chemistry Department of Centre for Research and Advanced Studies where she has been Academic Coordinater and Head of the Chemistry Department. Over 20 B. Sc., M. Sc. And Ph. D. students have carried out their final projects and tesis under her direction. She is a Member of te National System of Researchers foro ver 30 years and member of the Mexican Academy of Sciences and at present, she is a member of the directive council of this Academy. Member of several editorial committees. Part of diverse Evaluation Committees at Conacyt, UNAM and other institutions.

Primary author(s) : Dr. ROSALES HOZ, María de Jesús (Departamento de Química. CINVESTAV)

Presenter(s) : Dr. ROSALES HOZ, María de Jesús (Departamento de Química. CINVESTAV)

Session Classification : Guest Lecture

Contribution ID : **24** Type : **Presentation**

THE FUTURE OF SYNCHROTRON DATA COLLECTIONE

Saturday, 26 June 2021 12:30 (1:00)

Abstract

This talk will attempt to see into the future of synchrotron data collection with a focus on macromolecular crystallography (MX) but not forgetting other fields of research which are enabled by synchrotron radiation. MX is a field with a nearly 90 year history of which the last 50 years have included work at synchrotron X-ray sources. To enlighten my futuristic crystal ball, I will take a brief retrospective look at MX developments that have advanced the field and shaped current trends and practice. Recent breakthroughs such as those in protein structure prediction using AlphaFold2 [1] and the resolution revolution in cryo-electron microscopy [2] must be embraced when considering the future science best addressed by synchrotron radiation.

About

Elspeth graduated with a D.Phil (Ph.D.) in nuclear physics from Oxford Universityy in 1980 and switched to Biochemistry only later in her career, in 1987, when she joined the research staff at the Laboratory of Molecular Biophysics in Oxford. Since 1999 she has been faculty at the Biochemistry Department at Oxford University, where she holds a position as Professor of Molecular Biophysics and has also served as Director of the Systems Biology Programme at the Doctoral Training Centre. At Brasenose College she is a Nicholas Kurti Senior Research Fellow in Macromolecular Crystallography and until recently was Tutor for Graduates there. Elspeth's research on cryo-cooling and radiation damage has had a profound impact on crystallography. Armed with a rigorous approach inherited from her physics background and her natural inventiveness, she optimized cryogenic tools and cooling parameters, introducing a methodical approach to cryo-cooling that greatly improved diffraction data. Since radiation damage emerged as a serious problem in crystallographic structure calculation in 2000, she has spearheaded the studies dedicated to the issue, introducing mitigating measures such as the use of small molecules as radical scavengers. She experimentally determined the maximum x-ray dose that can be delivered to a macromolecule before compromising its structure -a parameter that is now called "the Garman" limit- and presented a method to predict the lifetime of proteins exposed to certain radiation doses. She also pioneered the use of an online UV-visible spectrometer to detect the early signs of radiation damage. Besides these studies, she developed the proton induced X-ray emission (PIXE) technique, which allows precise identification of trace metal elements within a protein structure, and she deternmined the structure of many proteins involved in infectious diseases.

Primary author(s) : Prof. GARMAN, Elspeth (Department of Biochemistry. University of Oxford)

Presenter(s) : Prof. GARMAN, Elspeth (Department of Biochemistry. University of Oxford)

Session Classification : Plenary Lecture

Contribution ID : **35** Type : **Poster**

Structural analysis of the partially disorder protein EspK by Small-Angle X-Ray Scattering

Wednesday, 23 June 2021 15:10 (0:10)

Abstract

For centuries, tuberculosis has been a worldwide burden for human health, and gaps in our understanding of its pathogenesis has hampered the development of new treatments. ESX-1 is a complex machinery responsible for the secretion of virulence factors that manipulate the host response. Despite the importance of these secreted proteins for pathogenicity, only a few of them have been structurally and functionally characterised. Here, we describe a structural study of EspK, a protein known to be essential for the secretion of other substrates and the cytolytic effects of ESX 1. SAXS data show that EspK is a large molecule with a maximal dimension of 228 Å. It consists of two independent folded regions at each end of the protein connected by a flexible unstructured region driving the protein to coexists as an ensemble of conformations. Limited proteolysis identified a small globular domain at the C-terminus of the protein consisting of a mixture of [U+F020][U+F061]-helices and [U+F062]-strands, as shown by CD and SAXS. In contrast, the N-terminal portion is mainly helical with an elongated shape. Sequence conservation suggests that this architecture is preserved amongst the different mycobacteria species, proposing specific roles for the N- and C-terminal domain assisted by the central flexible linker.

Primary author(s) : GIJSBERS, Abril (Maastricht Multimodal Molecular Imaging Institute, Maastricht University, Netherlands); SÁNCHEZ-PUIG, Nuria (Instituto de Química, Universidad Nacional Autónoma de México); SILIQI, Dritan (Institute of Crystallography-CNR)

Presenter(s) : SÁNCHEZ-PUIG, Nuria (Instituto de Química, Universidad Nacional Autónoma de México)

Session Classification : Poster Session

Contribution ID : **36** Type : **Poster**

Sistema de métodos y programas para caracterización de texturas axiales por difracción de luz sincrotrón y electrones

Wednesday, 23 June 2021 14:30 (0:10)

Abstract

Para dar una caracterización cuantitativa de la textura cristalográfica (caso de simetría axial) mediante la difracción de rayos X y electrones, el grupo de cristalografía de CIMAV desarrolló un sistema de métodos y algoritmos. El procedimiento que siguen los algoritmos consiste en dos líneas: Tipo método de Rietveld y tipo método de Bunge. Los inspirados en el método de Rietveld son ANAELU (ANAlytical Emulator Laue Utility) y GRAZING. En éstos, se modelan y refinan computacionalmente los patrones DRX partiendo de estructuras cristalinas y figuras inversas de polos (FIP) propuestas por el usuario. DIANNE (DIfracction ANalysis of Nanostructures with Electrons), el programa tipo método Bunge, se enfoca en el análisis de textura mediante la difracción de electrones y luz sincrotrón de alta energía. En el método seguido por DIANNE, se toman las figuras directas de polos (FDP) del experimento y se procesan con bases funcionales, obteniendo las figuras inversas de polos.

ANAELU representa una aproximación a un Rietveld bidimensional. Requiere un modelo estructura-textura inicial y conduce, mediante un ajuste entre los difractogramas bidimensionales (DRX-2D) calculado y observado, a una caracterización completa del policristal considerado.

En GRAZING la modelación de textura es sistematizada para obtener los DRX-1D para las geometrías Bragg-Brentano e incidencia rasante. Se aplica el modelo de textura al proponer una figura inversa de polos. Se compara el efecto de la textura en ambas geometrías.

DIANNE consiste en expresar los diferentes descriptores (FDP, FIP) en bases funcionales y relacionar los coeficientes de los desarrollos. La metodología consiste en ir de varias FP (unidimensionales) a la FIP (bidimensional) del eje de simetría de la muestra. DIANNE determina los coeficientes del desarrollo de las FDP en sus representaciones mediante series de polinomios de Legendre. Las FIP se consideran desarrollos en armónicos esféricos simetrizados. DIANNE calcula los coeficientes de la FIP a partir de los de las FP.

Primary author(s) : CAMPOS RODRÍGUEZ, Alejandro (Advanced Materials Research Center, 31136 Chihuahua, Mexico); FUENTES-MONTERO, Luis (Diamond Light Source Ltd); FUENTES-COBAS, Luis (Advanced Materials Research Center); NARVÁEZ MONROY, Juan (Advanced Materials Research Center)

Presenter(s) : CAMPOS RODRÍGUEZ, Alejandro (Advanced Materials Research Center, 31136 Chihuahua, Mexico)

Session Classification : Poster Session

Contribution ID : **37** Type : **Poster**

Synchrotron light in the structural studies of human transferrin for its application as a drug transporter in the central nervous system

Wednesday, 23 June 2021 14:40 (0:10)

Abstract

Human serum transferrin (Tf) is a ˜80 kDa glycoprotein that transits the blood plasma, whose function is to transport iron from its absorption site towards every cell through the blood vessels. Its structure consists of two homologous lobes, an N-terminal lobe and a C-terminal lobe, which can each bind a metallic ion, mainly Fe3+, through a coordination bond with octahedral geometry1–3. This important protein has been proposed as a potential drug transporter due to its transport mechanism across the blood-brain barrier4,5. To determine the feasibility of such system, a thorough structural and bioanalytical characterization of transferrin is essential, for which synchrotron light is a powerful resource. X-ray crystallography is one of the most widely used approaches for structure determination, and several Tf models have been obtained so far2,3,6–8; however, further research is necessary to generate high resolution models. Besides, a plethora of non-conventional crystallization techniques are available for crystal growth optimization, which in turn provides higher quality crystallographic data9–11. Therefore, the current project is exploring several of these methods for growing high quality transferrin crystals, being counter diffusion one of the main bets. Another powerful technique is Small Angle X-ray Scattering (SAXS), which has been able to provide information for Tf regarding its stability and behavior in solution12. Since transferrin's iron release mechanism has been shown to be pH dependent1, SAXS analyses at different pH conditions are being performed to study its conformation states throughout the stages of its iron binding and release cycle.

Primary author(s) : CAMPOS-ESCAMILLA, Camila (Institute of Chemistry, National Autonomous University of Mexico); SILIQI, Dritan (Institute of Crystallography (IC), National Research Council (CNR)); GAVIRA, José (Laboratorio de Estudios Cristalográficos, Instituto Andaluz de Ciencias de la Tierra (Consejo Superior de Investigaciones Científicas-Universidad de Granada)); GONZÁLEZ-RAMÍREZ, Luis (Laboratorio de Estudios Cristalográficos, Instituto Andaluz de Ciencias de la Tierra (Consejo Superior de Investigaciones Científicas-Universidad de Granada)); MORENO, Abel (Institute of Chemistry, National Autonomous University of Mexico)

Presenter(s) : CAMPOS-ESCAMILLA, Camila (Institute of Chemistry, National Autonomous University of Mexico)

Session Classification : Poster Session

Contribution ID : **38** Type : **Poster**

Mineralogical characterization and uranium radioactivity of recent sediments from the Laguna del Cuervo, Chihuahua

Wednesday, 23 June 2021 14:50 (0:10)

Abstract

The Sierra of Peña Blanca is found in the Aldama county region in the Chihuahua state, where most of the uranium natural deposits in Mexico are located. In the 1980s, mineral exploration was carried out with the molybdenum and uranium production by "Uranio de México (URAMEX)" company. However, in 1983, when the project was closed, the extracted and unprocessed ore was confined to rocky piles, exposing it to weathering. As a result, the runoff water that passes through the Peña Blanca reservoir accumulates at the bottom of the Laguna del Cuervo. Therefore, the mineral or dissolved uranium is transported and can potentially be deposited or precipitated in the sediments. In this work, the mineralogical characterization, the determination of the activity concentration of gamma-emitting radionuclides in a hyperpure germanium HPGe detector of the 238U radioactive series and the dating of a sedimentary core from the Laguna del Cuervo are exposed. It is recommended to apply a method to preserve the oxidation state of uranium in the samples, to be able to determine its speciation using X-ray absorption fine structure (XAFS) and X-ray photoelectron spectroscopy (XPS) techniques.

Primary author(s) : CARAVEO-CASTRO, Carmen del Rocío (Centro de Investigación en Materiales Avanzados (CIMAV)); MONTERO-CABRERA, María Elena (Centro de Investigación en Materiales Avanzados (CIMAV)); MÉNDEZ-GARCÍA, Carmen Grisel (Instituto de Física de la UNAM); CABRAL-LARES, Rocío Magaly (Centro de Investigación en Materiales Avanzados (CIMAV)); CASTILLO-SANDOVAL, Isai (Centro de Investigación en Materiales Avanzados (CIMAV))

Presenter(s) : CARAVEO-CASTRO, Carmen del Rocío (Centro de Investigación en Materiales Avanzados (CIMAV))

Session Classification : Poster Session

Contribution ID : **39** Type : **Poster**

Study of the Chemical, morphological and structural characteristics of Na-preconditioned Si anodes for lithium ion batteries by synchrotron techniques

Wednesday, 23 June 2021 15:00 (0:10)

Abstract

The current social challenges in energy storage have led to an increase in research to find new materials with improved characteristics to be used as anode in Li-ion batteries (LIBs) [1,2]. Silicon (Si) is one of the best candidates because of its high theoretical gravimetric capacity of 4200 mAhg-1, about ten times higher than that of graphite (372 mAhg-1). In addition, it is also the second most abundant material in the earth's crust, it is environmentally friendly and has a low electrochemical potential [3]. However, these benefits are accompanied by some drawbacks: (i) the insertion/extraction of Li+ from Si causes a large volume change ($> 300\%$); (ii) after a few cycles, Si may fracture (due to volume expansion) and pulverizes, causing loss of electric contact, which subsequently leads to severe capacity fade. To overcome these drawbacks and improve the stability of Si anodes, the use of nano- and micro-structured Si works. It has also been shown that cycling very slowly (10+ hours) for a few cycles (preconditioning process) before the normal use of the Si anode in a LIB helps to maintain mechanical stability [4,5]. In this work, an electrochemical preconditioning treatment was carried in Si anodes with Na. To observe in greater detail the modifications caused in the Si anodes due to the Na preconditioning treatment, synchrotron X-ray characterizations were used. The morphology of preconditioned Si particles was observed with ptychography. On the other hand, the different Si-Na phases formed during preconditioning, were evidenced through XRD (in situ and operando). Additionally, NEXAFS analysis provided information of the SEI formed on the Si anode.

Primary author(s) : ESPINOSA-VILLATORO, Erick (Institute of Physics, Benemérita Universidad Autónoma de Puebla (BUAP)); KO, Jesse (SLAC National Accelerator Laboratory); NELSON WEKER, Johanna (SLAC National Accelerator Laboratory); SANTILLÁN-GUZMÁN, Alina (Universidad Popular Autónoma del Estado de Puebla); QUIROGA-GONZÁLEZ, Enrique (Institute of Physics, Benemérita Universidad Autónoma de Puebla (BUAP))

Presenter(s) : ESPINOSA-VILLATORO, Erick (Institute of Physics, Benemérita Universidad Autónoma de Puebla (BUAP))

Session Classification : Poster Session

Contribution ID : **40** Type : **Poster**

Electron density contour maps via Rietveld-MEM analysis using HR-XRD for the polycrystalline ferroelectric BCZT

Wednesday, 23 June 2021 15:20 (0:10)

Abstract

The maximum entropy method in combination with the Rietveld refinement method applied to the analysis (Rietveld-MEM analysis) of high-resolution x-ray diffraction (HR-XRD) is an important tool to elucidate the electron density distribution and chemical bonding nature of materials. In this work, we present the comparison of electron density distribution obtained from the Rietveld-MEM analysis for polycrystalline perovskite BaTiO3 (reference sample) and Ba0.9Ca0.2Ti0.9Zr0.1O3 (BCZT). To perform this task, HR-XRD patterns using synchrotron radiation at the beamline 7.1 MCX of Elettra sincrotrone were acquired. Tetragonal phase with P4mm (No. 99) space group and pseudo-Voigt function were considered to model the HR-XRD peaks by the Rietveld method using the profile fitting Fullprof suite program. VESTA software was used to visualize 3D, 2D electron density distribution maps and line profiled to monitor the chemical bonding nature between Ba-O and Ti-O interactions and to visualize the off-center displacement of Ti cations by the incorporation of Zr and Ca cations. The interaction between Ti contours with O contours in the electron density distribution and the minimum electron density values revealed the enhancement of covalent nature and predominant ionic nature between barium and oxygen ions in the BCZT. To monitor the ferroelectric hysteresis behavior, polarization versus electric field curves complement the characterization of these samples.

Primary author(s) : HERRERA-PÉREZ, Guillermo (Catedra CONACyT assigned to Centro de Investigación en Materiales Avanzados (CIMAV)); PLAISIER, J. (Elettra-Sincrotrone Triestre); REYES-ROJAS, A. (Physics of Materials Department. Centro de Investigación en Materiales Avanzados (CIMAV)); FUENTES-COBAS, Luis (Physics of Materials Department. Centro de Investigación en Materiales Avanzados (CIMAV))

Presenter(s) : HERRERA-PÉREZ, Guillermo (Catedra CONACyT assigned to Centro de Investigación en Materiales Avanzados (CIMAV))

Session Classification : Poster Session

Contribution ID : **41** Type : **Poster**

Monte Carlo simulation of vacancies produced in lead-free piezo-ceramics by X-ray radiation damage

Wednesday, 23 June 2021 15:40 (0:10)

Abstract

Fourth-generation synchrotrons, such as ESRF – EBS (Extremely Brilliant Source) have a very high brilliance of 5x1022 photons / s / mm2 / mrad2 / 0.1% BW. This light is produced in pulses of very short duration, which allows experiments with high spatial, energetic and temporal resolutions. However, high brilliance produces huge beam intensities. This leads us to investigate whether the samples with a medium atomic number can be damaged during the experiments in the fourth-generation synchrotrons 1. These could be the case of experiments on ferroelectric materials. Radiation damage in ferroelectrics is reported in the literature. Among the consequences of ionizing radiation damage is the production of vacancies. Most of the studies have been carried out in PZT and using intense beams of X-rays, whose energy is much higher and the probability of interaction much lower than X-rays 2. This work presents the preliminary results of a simulation by the Monte Carlo method, performed through the GEANT4 code, of the irradiation of a BNBT6 ceramic with X-rays energies around the Ti-K absorption edge emulating a transmission experiment, and irradiation with 5300 eV X-rays for fluorescence measurement. The method consists of introducing the data that describe a characteristic R3c structure of the polarized ceramic, reported at Canche et al. 3. The absorption coefficients for the energies of interest, as well as the energy deposited in the form of radiation doses, are calculated. Intensity changes for specific energy lines in the micro-fluorescence spectra, which suggest the presence of vacancies in the crystal structure, are verified via simulation. The vacancy density produced by a typical photon flux of a fourth-generation synchrotron beam is calculated through the vacancy formation energy. Consequently, the simulation is carried out for a structure with appropriate Bi and O vacancies, and the ability to detect the radiation damage is verified by comparison with XRF and XAFS experimental results 3. The support provided by Project CONACYT Projects No. 183706 and 257912, as well as MINECO MAT2017-86168-R, Spain, is acknowledged. A part of the experiments was performed (as part of Proposal No. 3511) at the Stanford Synchrotron Radiation Lightsource (SSRL). XAFS experiments were accomplished at the European Synchrotron Radiation Facility (ESRF) at Grenoble, as part of the proposal HG/77.

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Session Classification : Poster Session

Contribution ID : **42** Type : **Poster**

CO2 sensing mechanism of ZnO & ZnO/MWCNT

Wednesday, 23 June 2021 15:50 (0:10)

Abstract

Nowadays, sensing devices to monitor CO2 concentrations in human exhalation and the environment are essential to identify acceptable limits, including ventilation rates in workplaces in order to optimize the return to classrooms, laboratories and offices during the global coronavirus pandemic (SARS CoV[U+2010]2). In this study, we combined ZnO and MWCNTs to obtain a composite material and analyze their structural, and sensitive properties. In this work, pure ZnO nanostructures were synthesized by homogeneous precipitation with hexamethylenetetramine (HMTA) as precipitation agent. MWCNT used in the experiments were prepared by spray pyrolysis at 700 ºC. A nanocomposite of zinc oxide and multiwall carbon nanotubes (ZnO-MWCNT) was prepared by spray pyrolysis. The samples were tested in various concentrations of CO2 atmospheres ranging from 5 to 500 ppm. The Synchrotron X-ray (SXRD) measurements were carried out at room temperature confirming the hexagonal wurtzite phase of ZnO and composite. Raman analysis shows the detailed structural and significance differences between both ZnO and ZNO-MWCNT samples. SEM analysis indicated the rod-like morphology of ZnO structures and the agglomerates prisms of ZnO-MWCNT nanocomposite samples. Moreover, the CO2 detection properties like sensing response, response time, recovery time, repeatability, and stability for both the samples were obtained and discussed in detail. Finally, selectivity analysis with respect to acetone and ethanol were performed and corresponding gas sensing mechanisms are reported in this work.

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Session Classification : Poster Session

Contribution ID : **43** Type : **Poster**

Influence of sunlight and atmospheric pressure on the synthesis of Ca (II), Ba (II) and Sr (II) silica-carbonate biomorphs

Wednesday, 23 June 2021 15:30 (0:10)

Abstract

To explain and understand the chemical origin of life, theories have been postulated for decades and some of them have gone from mere postulates to evidences that have contributed to science in this direction. Several research groups have developed study models elucidating which could have been the first forms of life; in this sense, calcium, strontium, or barium silica carbonates have been synthetized in vitro that emulate morphologies of organisms. Aimed at understanding better the influence of sunlight and atmospheric pressure in the formation of different chemical structures, the importance of the different types of physical abiotic factors in the origin of life are reviewed, as well as their influence on the morphology of biomorphs.

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Session Classification : Poster Session

Contribution ID : **44** Type : **Poster**

Naica's Giant Crystals: Characterization by synchrotron radiation of the wall-crystal interface

Thursday, 24 June 2021 16:00 (0:10)

Abstract

Naica´s "Cueva de los Cristales" was discovered in 2000, and since then it has been considered particularly interesting for its beauty and for the challenges it poses to crystallography. This article focuses on the study of the wall-selenite interface by various techniques, particularly X-ray diffraction (XRD), scanning electron microscopy (SEM), with emphasis on micro-X-ray fluorescence ([U+F06D]-XRF) and micro-X-ray absorption near edge structure ([U+F06D]-XANES). The main phases calcite, quartz, goethite and montmorillonite were identified by XRD, as well as the association of crystalline and amorphous minor and trace phases of Zn, Mn, Cu, As and Pb. The later were identified in [U+F06D]-XRF maps and [U+F06D]-XANES spectra. The results for the morphology and the chemical description of the crystal-wall interface may contribute to propose a nucleation and growth mechanism for Naica megacrystals.

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Session Classification : Poster Session

Contribution ID : **45** Type : **Poster**

Uranium isotopes concentration and transport in the Laguna del Cuervo, Chihuahua, Mexico.

Thursday, 24 June 2021 14:40 (0:10)

Abstract

In Chihuahua, an important source of environmental radioactivity is found in the Sierra Peña Blanca, in the center of the state. The site has about 70% of uranium reserves in Mexico. The uranium of Peña Blanca was exploited in the 80's. Due to the closure of operations, the extracted and unprocessed ore (hundreds of tons) was confined to rocky stacks, exposed to weathering. Subject to leaching, this uranium is transported from the mountains to Laguna del Cuervo. The mineral exposed in the repository and the uranium transport by water and recent sediments must be studied, to assess the effects on the environment, with radiometric and materials science techniques in conventional laboratories and synchrotron light. This work presents the study of sediment and pore water samples at various points along the lagoon, and the values of the activity ratio of the 234U/238U isotopes and the sediment-water distribution coefficient of these isotopes, obtained by applying uranium liquid scintillation alpha spectrometry, gamma-ray spectrometry, scanning electron microscopy and X-ray diffraction methods.

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Session Classification : Poster Session

Contribution ID : **46** Type : **Poster**

Molecular characterization of bacteria to oxidize As(III) for water treatment in rural communities; study case Xichu, Guanajuato. Mexico

Thursday, 24 June 2021 14:50 (0:10)

Abstract

Arsenic (As) concentration of 98 μg L-1 was found in Xichu River waters, which exceed the limits established by the WHO and the Mexican normativity NOM-127. This concentration is a potential risk for the population. It is necessary the search of available technology to remove As form drinking water in the most affected regions (rural communities), due to socioeconomic situation which they are in. In addition, at the same time disables them to implement a conventional As removal treatment. Bioremediation of water using As resistant bacteria-based technologies may provide a better alternative. Through the application of statistical analysis it was possible to corroborate the capacity of three bacteria strains to growth in As(III) stress conditions: Rhodoccocus gordoniae, Microbacterium hydrocarbonoxydans and Psedomonas kribbensis. The presence of aox genes was corroborated in 2 strains. PHB production could represent a value-added sub-product after a biological stress, e.j., biological treatments. In this study, it is proposed the use of synchrotron techniques to identify the localization of the As transformation either intracellular or extracellular, and the observation of possible compounds in the cellular membrane that can interact with As(III) by biosorption or bioaccumulation. Moreover, these synchrotron techniques may help to study the As speciation in water samples and in media culture before and after bacteria interaction. Some synchrotron techniques such microscopies (SEM/EDS), microespectroscopy (SR-FTIR) and XAS (X-ray Absorption Spectrospy) are proposed for further studies.

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Session Classification : Poster Session

Contribution ID : **47** Type : **Poster**

Fine structural disorders in nanostructured TiO2 films for photovoltaic applications.

Thursday, 24 June 2021 15:00 (0:10)

Abstract

Abstract: In the last years, interest on renewables energies has increased and solar energy is one of most promising alternatives to get clean and worldwide available energy. Photovoltaic devices have been designed and applied to convert photons coming from Sun into electrons. Dye-Sensitized Solar Cells (DSSCs) are a good example because of its low-cost fabrication and good performance reaching about 12% efficiency conversion. However, DSSCs presents several problems like poor stability. Several methods and novel materials have been studied to improve DSSCs' stability, for example, changing the dye molecules´ structure to improve dye-attachment to the TiO2 surface and substituting liquid solvents in the electrolyte solution for quasi-solid-state electrolytes. These improvements have been studied from photovoltaic and electrodynamical point of view and corelated with changes on the TiO2 surface in somehow, however, these studies have not proven yet if there are a relationship between the observed photovoltaic and electrodynamical behaviors and changes on the TiO2 lattice. As starting point, in this work, we studied the changes on TiO2 nanostructured films when they are compared with an ideal TiO2 structure, i.e., bulk sample. Our results indicates that a nanostructured sample results in a more stressed and disorder crystal network than the lattice from the bulk sample, these characteristics have been related with the increase of oxygen vacancies at the TiO2 surface, known as energy traps.

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Session Classification : Poster Session

Contribution ID : **48** Type : **Poster**

Development of HAp/TiO2 Composites for the preparation of Piezoelectric Biomaterials

Thursday, 24 June 2021 15:10 (0:10)

Abstract

Bone is the second most implanted tissue only after blood, therefore the interest in developing new biomaterials that replace the functions of bone and cartilage are of great interest today. Hydroxyapatite, bioactive and piezoelectric ceramic, is the most common biomaterial used for bone tissue and it demonstrates that the incorporation of metallic oxides such as titanium oxide (TiO2), reflects an improvement in mechanical properties that it lacks by itself. On the other hand, properties such as pyroelectric, ferroelectricity and piezoelectricity of HAp have been a subject of great interest in the regeneration of bone tissue. In this work nanocomposite powders were obtained by co-precipitation and sol-gel methods assisted by ultrasonic radiation, using Ca (NO3)2 • 4H2O and (NH4)2 HPO4 as precursors of HAp and TiOSO4 • xH2O as precursor of TiO2. The Synchrotron X-ray (SXRD) and STXM measurements were used to determine the crystal structure, environmental composition and formation of the composite. The HAp/TiO2 composite was formed and showed a mixture of phases. PFM measurements of composite indicated a good agreement with effective piezoelectric constant. The composite obtained exhibits piezoelectrical and mechanicals properties that can be used in the manufacturing of scaffolds either as support in fractures or in conjunction with collagen for the regeneration of bone tissue.

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Session Classification : Poster Session

Contribution ID : **49** Type : **Poster**

Characterization of As remotion mechanisms in a natural limestone filter

Thursday, 24 June 2021 15:20 (0:10)

Abstract

The present work proposes an effective methodology to remove arsenic (As) present in groundwater for human consumption. Column experiments carried out with limestones outcropping in a groundwater As-rich area were found to effectively remove As, and have been considered as a sustainable treatment option. The study is focused on the aquifers at Zimapán town, Hidalgo, México, where the As concentrations rises values up to 1.2 mg/l, that surpass up to 48 times the permissible limit according to the Mexican regulation for drinking water (NOM-127-SSA1-2000) and 120 times the reference value according to the World Health Organization (WHO) [1,2]. The limestone material was characterized by means of X-ray diffraction (XRD) and X-ray fluorescence (XRF). Batch tests were performed using CaCO3 (reagent grade) with different arsenic solutions (50 ppm, 300 ppm, and 12000 ppm) as reference standards and testing experiments. Accordingly, it was necessary to apply high-resolution techniques such as synchrotron light radiation, specifically X-ray absorption spectroscopy (XAS) to unsolved involved mechanisms. These XAS spectra at As K-edge were collected in the Elettra Sincrotrone Trieste for references and experimental columns. Linear Combination Analysis results showed that in all samples, the main As removal mechanism is adsorption, with more than 90%; and less than 10%, we find: (1) precipitation of As with Ca, (2) with Na, and (3) retained As associated with Fe. Overall, the experiments indicated that home-filters based on these limestones may be developed to use as an alternative to avoid population exposure, mostly in isolated small communities.

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Session Classification : Poster Session

Contribution ID : **50** Type : **Poster**

Synchrotron-FTIRs studies of microbially-mediated biomineral formation

Thursday, 24 June 2021 15:30 (0:10)

Abstract

Biomineral formation is a key process to understand the linkage between biological activity and sedimentary structures in the biosphere. Microbial systems have mediated the precipitation of carbonates in natural waters as early as $\sim$ 3,500 Ma ago (Krumbein 1983); and still today they are key participants in the formation of massive carbonate constructions in natural waters. Microscale has been a relevant challenge to understand biomineral formation. This research has been invigorated recently by using advanced imaging technologies, such as Synchrotron based-Fourier Transform Infrared spectromicroscopy (SR-FTIRs). This is a non-labelled, non-destructive, spatially resolved strategy that allows chemical characterizations of live cells with microscale resolution. SR-FTIRs revealed structural and functional features of microbial-only biomineral forming systems (microbialites) but also of host-microbiota systems (coralline algae). These first results provide insight into the characteristics of the microsites of mineral formation, and are useful to inspire bio-cement development and carbon sequestration technologies in an increasing CO2 world.

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Session Classification : Poster Session

Contribution ID : **51** Type : **Poster**

Una representación de las secciones de Poincaré para la dinámica de partículas en la estructura magnética de un acelerador usando cuasi invariantes de movimiento aproximados

Wednesday, 23 June 2021 16:00 (0:10)

Abstract

El diseño de aceleradores de partículas es un área de investigación muy activa en los últimos años. Dependiendo del fin de la máquina, ajustar la dinámica de las partículas en la estructura magnética puede representar un problema no trivial. Es bien sabido que el análisis de la geometría del espacio fase, así como su dependencia con los parámetros del hamiltoniano, resulta complicado para estos sistemas. El objetivo de este trabajo es desarrollar una herramienta analítica para estudiar localmente la estructura geométrica del espacio fase de sistemas hamiltonianos no autónomos no lineales, en regiones no caóticas y alejadas de resonancias intensas. Para estas condiciones, y haciendo uso de cuasi-invariantes representados por medio de series de potencias de las coordenadas y los ímpetus generalizados asociados, mostramos una representación aproximada de las secciones de Poincaré de dichos sistemas. La forma polinomial de estos cuasi-invariantes aproximados, a un orden dado, nos permite elegir la precisión con la que el espacio fase es descrito, además, por medio de ellos, el problema de resolver las ecuaciones de movimiento es reformulado en términos de la solución de un problema algebraico. Como ejemplo, analizamos uno de los cuasi-invariantes del hamiltoniano asociado a una lattice de un modelo posible para el Sincrotrón Mexicano. Este método de análisis puede ser muy útil en aquellos casos en los que se prescinde de las soluciones, exactas o aproximadas, de las ecuaciones de movimiento de estos sistemas.

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Session Classification : Poster Session

Contribution ID : **52** Type : **Poster**

Chemical speciation of lead adsorbed onto volcanic ashes by ICP-OES and XANES

Thursday, 24 June 2021 15:40 (0:10)

Abstract

This study focuses on the assessment of the VA materials from the Moungo zone of the Cameroon volcanic line (CVL) between the mount Cameroon volcano and Mount Koupé, for their use as natural adsorbent to remove Pb(II) pollutant from aqueous solutions. The chemical speciation of lead adsorbed onto volcanic ashes based by means of X-ray absorption near edge spectroscopy (XANES) study is reported. The ashes from Cameroon volcanic line in the Moungo zone (Littoral-Cameroon) are used to remove lead in aqueous solutions. The maximum value of the adsorption capacity of lead in volcanic ashes was 7.60 mg g-1 at pH 5. Regarding the adsorption process, the contribution of the mixture lead components after adsorption and a strong interaction of adsorbed lead with the surface of volcanic ashes were proven. The chemical elements present in the volcanic ash and their concentrations are determined by inductively coupled plasma optical emission spectroscopy (ICP-OES). Chemical speciation was carried out measuring unsaturated, and Pb saturated volcanic ash samples around at the L3 edge (13035) at the XAFS beam line in Elettra Sincrotrone Trieste. The XANES measurements showed that the lead removal occurred mainly by microprecipitation of lead acetate and carbonate (cerussite). In addition, a possible ion exchange is also involved forming lead monoxide.

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Session Classification : Poster Session

Contribution ID : **53** Type : **Poster**

Distribution and chemical speciation of Pb in agricultural soils near a mine tailing deposit in northwestern México

Thursday, 24 June 2021 15:50 (0:10)

Abstract

Management of industrial residues is a growing concern all around the world. In Mexico and specially in Sonora, mining is one of the most active and economically relevant industries, associated with environmental problems. Mine tailings contain potentially toxic elements (PTE), that are dispersed during long periods of time by erosion and weathering processes of the minerals they are in and suffer chemical transformations, that in turn, mediate the mobilization to other environmental compartments. This study focused on the agricultural soils near the mine tailings in San Felipe de Jesús, Sonora. For this, the presence of Pb in the tailings and agricultural soils was quantified, using inductively coupled plasma mass spectroscopy (ICP-MS) and X-Ray fluorescence (XRF). Physicochemical parameters were measured as indicators of Pb presence (pH, EC, real density). Anthropogenic pollution using the geoaccumulation index (Igeo) was calculated and the parameters were analyzed using geostatistical and GIS software (ArcGIS) to visualize its distribution in the study area. The mineralogy and chemical species were carried out using XRD, scanning electron microscope with an energy dispersive detector (SEM-EDS) and X-Ray absorption spectroscopy (XAS) using synchrotron light. The main results showed that Pb concentrations exceed mexican regulations and concentration maps suggest a possible mobilization by water associated to "El Lavadero" creek and a negative spatial correlation with pH values. Pb rich jarosite was identified and a correlation between Pb and S in oxidized pyrite crystals was observed which may indicate a relation with its mobilization. Additionally, Pb can mainly be found with an oxidation state of Pb2+. Agricultural soils and mine tailings contain chemical species of Pb with structures like massicot and galena, with a minor presence of beudantite, cerussite and anglesite like structures. The species associated to its mobility are beudantite, cerussite and anglesite.

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Session Classification : Poster Session

Contribution ID : **54** Type : **Poster**

Characterization of pellets from lignocellulosic waste for use in the treatment of water contaminated with Metals and Metalloids

Thursday, 24 June 2021 16:10 (0:10)

Abstract

The characterization of pellets of lignocellulosic residues from different crops of the Xichú, Gto. Different values of humidity were obtain like 4.58%±1%, eliminated organic material, remainder and total 45.36% ±4 %, 39.84% ±3% and 85.17% ±4.5% respectively, and inorganic material (ashes) 14.83% ±2%. These preliminary studies contribute to the possibility of the use of lignocellolosic inside the prototypes designed in order to make the quality of the water in the region of Xichu Gto better.

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Session Classification : Poster Session