



**SECOND MEXICAN SYNCHROTRON RADIATION USER'S MEETING  
(MESYRUM 2012)**

**June 6-8th, 2012, León, Guanajuato, México**

**BOOK OF ABSTRACTS**



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Dr. Erick Adrián Juárez-Arellano (Universidad del Papaloapan, Oaxaca).



## Second Mexican Synchrotron Radiation User's Meeting (MESYRUM2012)

### PROGRAM

	Wednesday 6			Thursday 7		Friday 8
8:30-9:00	Registration		8:30-9:00		8:30-9:00	
9:00-9:30	Opening		9:00-9:30	<b>IT2:</b> Vivian Stojanoff (Brookhaven National Laboratory, USA)	9:00-9:30	
9:30-10:00	<b>IT1:</b> Harald Reichert (European Synchrotron Radiation Facility, EU)		9:30-10:00		9:30-10:00	<b>S7:</b> Iris Selene Gómez (UAZ)
10:00-10:30			10:00-10:45	<b>C5:</b> Enrique Rudiño (UNAM)	10:00-10:30	<b>IT4:</b> Chris Jacobsen (Argonne National Laboratory-Notwestern University, USA)
10:30-11:15	<b>C1:</b> Maria Elena Montero (CIMAV)		10:45-11:15	<b>S5:</b> Irma Robles (CIDETEQ)	10:30-11:00	
11-15-11:45	Coffee break	Meeting ESRF Room A	11-15-11:45	Coffee break	11-00-11:30	Coffee break
11:45-12:30	<b>C2:</b> Paola Zapata (UAZ)		11-45-12:45	<b>IT3:</b> Hiram Castillo Michel (ESRF, EU)	11-30-12:00	<b>S8:</b> Eunice Yañez (UG)
12:30-13:15	<b>C3:</b> Jesús Alvarado (UNAM)		12:45-13:30	<b>C6:</b> Rene Loredo-Portales (UG)	12:00-12:30	<b>S9:</b> Adolfo López Torres (UG)
13:15-13:45	<b>S1:</b> Hugo A. Sandoval (UAZ)		13:30-14:00	<b>S6:</b> Gladys Morales (UG)	12:30-13:15	<b>C10:</b> Gustavo Cruz (UG)
13:45-16:00	Lunch		14:00-16:00	Lunch	13:15-14:00	<b>C11:</b> Gilberto Gutiérrez (UG)
16:00-16:45	<b>C4:</b> Ibrahim Serroukh (Universidad Autónoma de Querétaro)		16:00-16:45	<b>C7:</b> J.C. Fierro González (Ins.Tec. de. Celaya)	14:00-14:30	<b>S10:</b> Ana Kotanjan (Yerevan State Univ. Armenia)
16:45-17:15	<b>S2:</b> Esteban Rivera Pérez (UAZ)		16:45-17:30	<b>C8:</b> Erick A. Juarez Arellano (Univ. Papaloapan)	14:30:00	Closing.
17:15-17:30	Coffee break		17:30-17:45	Coffee break		
17:30-18:00	<b>S3:</b> Hector Asael de León (UAZ)		17:45-18:30	<b>C9:</b> Michelle Alvarez (ESRF)		
18:00-18:30	<b>S4:</b> Flavio Manuel Nava (UAZ)					
20:30-23:30			20:30-23:30	<b>Dinner</b>		



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**BOOK OF ABSTRACTS**

**Wednesday, June 6th**

**IT1: "Science with Synchrotron Radiation from a 6 GeV Source", Harald Reichert, European Synchrotron Radiation Facility. EU.**

The European Synchrotron Radiation Facility is the only international synchrotron radiation facility. Constructed about 20 years ago as the world's first 3rd generation hard x-ray source, the facility is currently engaged in an ambitious upgrade program covering all aspects of hard x-ray photon science: photon production, experimental facilities for users, user service, and x-ray technology development. The upgrade has been designed around five scientific key drivers and benefits all x-ray techniques: Imaging, Spectroscopy, and Diffraction. As the upgrade program is producing its first deliverables, examples of recent experiments will be used to demonstrate the potential which modern synchrotron radiation sources offer for fundamental and applied sciences. Especially for applied sciences and innovation, we have put forward efforts to attract new user communities. Examples from applied geosciences and the wide field of structural materials will be used to prove the synchrotron's potential in this area.

**C1: "Selenite giant crystals at Naica: study of environmental effects", Maria Elena Montero Cabrera, Centro de Investigación en Materiales Avanzados, México.**

Inside a Pb (760000 ton/y), Zn and Ag mine at Naica, Chihuahua, are the largest selenite (gypsum- $\text{CaSO}_4 \cdot 2\text{H}_2\text{O}$ ) crystals over the World. Naica large crystals are well known since 1910, when the so-called Cave of Swords was discovered. In 2000 year a chamber was discovered at 290 m underground, in the Cueva de los Cristales (Giant Crystals Cave). This cavern contains gypsum crystals as long as 11 m and as thick as 1 m, which are much larger than any gypsum crystal previously reported. The formation of giant crystals was explained in (Garcia-Ruiz, Villasuso et al. 2007). Giant crystals have their value inside the cave, and not in external museums. Under the criteria of the UNESCO World Heritage Convention, the Giant Crystal Cave could be considered as a "World Natural Heritage of Outstanding Universal Value". A general project on the site has to be developed for making this officially supported by state and federal governments. This project includes a scientific project for the conservation and exhibition of the giant crystals. Surface composition determination using grazing incidence + area detector XRD and XPS; optical and physical characterization of Naica crystals (confocal microscope, refratometry); characterization of environmental modification of crystals during atmospheric changes and predictive models and simulation of crystal changes in different scenarios, are included in the project. The first results on

grazing incidence and transmission X-ray diffraction, performed on selenite crystals from the Cave of Swords and Giant Crystals, are presented in this talk. Experiments were done at Stanford Synchrotron Radiation Lightsource. In the transmission pattern, selenite single crystal reflections are identified. On a polluted surface of a crystal from the Cave of Swords the initial interpretation given is: on the Gypsum bulk, calcite, hematite and syngenite are present as additional lower concentration phases. All diffraction peaks have qualitative interpretation.

Keywords: grazing incidence XRD, Giant Crystals, Naica.

References: Garcia-Ruiz, J. M., R. Villasuso, et al. (2007). "The Formation of Gypsum Megacrystals." *Geology* 35(4): 327-330.

**C2: Relationship Between Obesity and Insuline Resistance in Patients From Zacatecas Mexico.** Paola Guadalupe Zapata Rodríguez, Unidad Académica de Estudios Nucleares, Univ. Autónoma de Zacatecas, México.

The state of Zacatecas in Mexico occupies the national second place in obesity where the incidence is higher in adults, even if increasingly more younger adults whose show this kind of problem; thus, it could trigger another diseases as diabetes mellitus and arterial hypertension. The first references about insulin resistance were made by Himsworth in 1936, when he referred to insulin-resistant and insulin-sensitive diabetic people. The insulin resistance, as primary pathogenic event in the diabetes mellitus type 2 (DM2), is derivate from the obesity, that implies a subnormal biologic response in the metabolism of carbohydrates, proteins and lipids. In this study we made a quantification of insulin levels by Radioimmunoassay (R.I.A.) in forty obese patients with evident obesity and eight normal weight patients accord to their age and abdominal circumference. There were three statistic correlations for both groups (obese and normal weight patients). The first ratio indicates the waist size with insulin quantity secreted, and accords the obtained results, this correlation is higher in all patients, that means there are a big dependence between waist size and the insulin quantity that they have. The second correlation was between age and insulin quantity secreted; the result of the correlation indicates that, even this relation is small, there are no matter the age for insulin secreted. The third and last correlation was between age with waist size, and the results showed that there exist correlation, but not as significant as the first correlation. Therefore, it is concluded that there are a very significant relationship between obesity and insulin resistance.

**C3: Non-invasive study of fossils preserved in Chiapas amber using Synchrotron-based Infrared and X-ray fluorescence microspectrometry.** *Jesus Alvarado Ortega, Francisco Riquelme, Instituto de Geología, Universidad Nacional Autónoma de México; José Luis Ruvalcaba, Instituto de Física, Universidad Nacional Autónoma de México.*

Synchrotron light source produce infrared photons using in microspectroscopy to characterize both organic and non-organic materials with size close to the diffraction limit. Synchrotron IR photons are too large in energy (0.05-0.5 eV) to break any chemical bonds or cause ionization, also produce minimal heating of the samples and generate spectra with high signal to noise ratios in spatial resolution between 3-10  $\mu\text{m}$ . Additionally, Synchrotron

X-ray fluorescence is a non-destructive microspectroscopy used to fully map trace element distribution in samples which require little or no pretreatment. Also provides some advantages, including wide elemental coverage with a typical sensitivity of  $\mu\text{g/g}$ , as well as making in-situ analysis and testing small-scale areas with a beam flux from 4.5 to 32 KeV and spot size as fine as 15-10  $\mu\text{m}$ . Thus, the IR and XRF synchrotron-based techniques using U2b, X15a and X27a beamlines from the National Synchrotron Light Source (BNL) has been successfully developed to study hard and soft tissues of fossils exceptionally preserved in amber from the Early Miocene Chiapas deposits (ca. 23 Ma.), Southern Mexico. Results show highly conserved ancient biological tissues in plants and animals and evidence of the diagenetic geomolecular transformation occurred to tissues and biomolecules induced by fossilization process, as well as the chemotaxonomic signal of the plants associated with the amber production.

**S1: Effect of Humic Acid on the Sorption of U(VI) onto Mexican Natural Zeolite.** *Hugo Apolonio Sandoval García*, Universidad Autónoma de Zacatecas

It was studied the uranium sorption onto a mexican natural clinoptilolite zeolite in presence and absence of humic acid (HA). Kinetics sorption and pH effect in the binary U-zeolite and ternary U-zeolite-HA systems were studied. Also it was investigated the behavior of HA-coated zeolite on the removal of uranium as a function of pH. The experiments were carried out uranium and HA concentrations of  $1 \times 10^{-5}$  M and 20 ppm, respectively, and a m/V ratio of 5 mg/mL. Uranium sorption in absence of HA was 95%, and it was reduced to 45% in the ternary system U-zeolite-HA. The results of the binary system U-zeolite were analyzed by applying three sorption kinetic models (pseudo-first order, pseudo-second order and Elovich). By using nonlinear regression it was found that uranium sorption follows a pseudo-second order kinetic. Metal sorption in the binary U-zeolite and ternary U-zeolite-HA systems was enhanced at low pH and decreased as pH increases. However uranium sorption onto HA-coated zeolite was found to be favored at pH above 5.

**C4: EDXRF and application to art pieces and biological materials,** Ibrahim Serroukh , Universidad Autónoma de Queretaro.

This work present the advances and interest of the collaboration Guanajuato-Queretaro in the study of art pieces and biological materials. The main technique in use is the EDXRF spectroscopy. This technique can be used for rapid evaluation of samples, in synchrotron studies. Also, this technique can report a rapid analysis about the elemental composition and the corresponding concentrations. Such information is valuable in the programing of energies and intensities in the synchrotron line, for material sciences studies.

**S2: Design and evaluation of a poliethylene cilynder for using in the AXAN using the photoneutrons of a 15 MV LINAC.** *Esteban Rivera Pérez*, Universidad Autónoma de Zacatecas.

When a linear accelerator of medic use operate above 8 MV photonuclear reactions are produced like ( $\gamma$ , n), the produced neutrons present a radiological risk both for the patient and the staff. So far, these neutrons are considered undesirable because it increases the dose to the patient. The aim of this work is to take advantage of the field of photoneutrons

produced by a linear accelerator to performed the NAA in small samples, for which was designed a moderator medium using Monte Carlo methods and evaluated their performance in a 15 MV LINAC when 4 solutions of manganese in different concentrations were irradiated, besides of determining the activity induced in pieces of Au of different dimensions.

**S3: Radioisotopes induced in samples of concrete inside the treatment hall with a LINAC for radiotherapy.** *Hector Asael de León Martínez*, Universidad Autónoma de Zacatecas.

When linacs operate above 8 MV an undesirable neutron field is produced, due to room-return effect inside the room there is a thermal neutron flux that is constant and when these thermal neutrons collide with the bunker walls some radioisotopes are induced in the concrete. In aim of this work is to study the induced radioisotopes in concrete samples which emit gamma-ray during its decay, the presence of these photons will represent a radiological risk for the patient. The mean peaks resultant in this work was Al, Na and Mn and there were similar results for all the samples.

**S4: Determination of Th y U by Neutron Activation Analysis for Gamma in Situ Spectrometry Calibration.** *Flavio Manuel Nava Maldonado*, Unidad Académica de Estudios Nucleares, Univ. Autónoma de Zacatecas, México.

Using Neutron Activation Analysis, U and Th depth distribution profiles were determined, calibration factors were obtained for use in Gamma ray in Situ spectrometry. Three site of Zacatecas state were sampled and Neutron Activation Analysis was carried out in Nuclear Engineering Teaching Laboratory of University of Texas at Austin with nuclear reactor TRIGA. From the Gamma in Situ spectrums, photopeak areas were obtained and normalized for radionuclides Tl 208 and Ac 228 for Thorium and Pb 214 and Bi 214 for Uranium serie. Factor averages with units cpm/Bq/Kg of 105.63 +- 8.32 and 75.87 +- 4.61 for Th and U respectively were found.

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**Thursday, June 7th**

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**IT2: The beauty in synchrotron radiation.** *Vivian Stojanoff*, Brookhaven National Laboratory, USA.

From the analysis of ancient artifacts to today's complex DNA molecular structures synchrotron radiation in the form of infrared, ultraviolet and x-ray light has shed light on innumerous subjects contributing to the better understanding and characterization of materials as simple as silicon to molecules as complex as the ribosome. In this presentation we will discuss those techniques that are particularly well adapted to the analysis of the molecular structure, chemical analysis, and imaging.

**C5: Crystallographic Evidence for Proton-Relay Mechanism in the O<sub>2</sub> Reduction to H<sub>2</sub>O by a multicopper oxidase from *Thermus thermophilus* HB27.** *Enrique Rudiño Piñera*, Instituto de Biotecnología- UNAM.

*Thermus thermophilus* multicopper oxidase (Tth-MCO) catalyzes four one-electron oxidations of reducing substrates and coupled this to the four-electron reduction of molecular oxygen to water. During X-ray data collection of a multicopper oxidase crystal, electrons are released and photoreduction of copper atoms seems to take place leading to the reaction of bound molecular oxygen to water. In fact, the final crystallographic structure is a mixture of several copper and neighboring residues oxidation states and molecular oxygen to water intermediaries. This study focuses on two different crystallographic strategies in order to study the proton-relay mechanism in reductive cleavage of the O<sub>2</sub>, and the role of Glu451 and Asp106 residues of the Tth-MCO in this mechanism. First, we report the structure of the Tth-MCO at 1.5 Å resolution and two inactive forms of the enzyme, apo-Tth-MCO and Hg-Tth-MCO, both at 1.7 Å resolution. Second, we describe a multicrystal data collection strategy and present a three-dimensional movie of the X-ray O<sub>2</sub> induced reduction, in which eight structures of the Tth-MCO at 1.8 Å resolution with different X-ray absorbed doses were obtained by combining data from eight Tth-MCO crystals. In the latter case, we obtained composite data sets, trapping different intermediaries of the O<sub>2</sub> reduction to water. In addition, the crystallographic evidence of the role of Glu451 residue providing protons to the catalytic reaction at the trinuclear copper center of the enzyme was ratified. Finally the high susceptibility of T2Cu in relation with the remaining coppers atoms is stress, probing that at doses higher than 2.5 MGy the depletion of this atom is complete.

**S5: Electroremediation of Mercury Polluted Soil by Removing Agents.** *Irma Robles*, Centro de Investigación y Desarrollo Tecnológico en Electroquímica, Cideteq, México.

Electrochemical remediation has been recognized as a promising technology to address difficult contaminated soil conditions. The goal of this technique is to affect the migration of subsurface contaminants in an imposed electric field via electroosmosis, electromigration, and/or electrophoresis processes. Electrochemical removal of heavy metals needs to be enhanced due to chemical composition, higher buffering capacity, and different metal speciation. One enhancement strategy is the use of complexing agents. Electroremediation of mercury polluted soil, facilitated by the use of complexing agents, proved to be an attractive alternative treatment for the removal of mercury from polluted soil in mining areas located at the Sierra Gorda in Querétaro, Mexico. Implementation of this remediation protocol is expected to improve the living conditions and general health of the population in this region. Experimental observations suggest that it is possible to remove up to 75 % of metal contaminants in mercury polluted soil samples by wetting them with 0.1 M EDTA, placing them in an experimental cell equipped with Ti electrodes, and then applying a 5 V electric field for 6 hours. The efficient removal of mercury contaminants observed under these conditions is attributed to electromigration of the coordination complexes that form between the terminal hydroxyl groups in EDTA and divalent mercury (Hg<sup>+2</sup>). This interaction is probably strengthened by supramolecular interactions between unshared electrons at EDTA's tertiary amino nitrogen and Hg<sup>+2</sup>. Speciation of mercury in soil can be achieved by using analytical techniques such as Synchrotron Radiation.

**IT3: The ID21 beamline at the European Synchrotron Radiation Facility: an ideal tool for sub-micrometric 2D speciation analyses.** *Hiram Castillo-Michel, European Synchrotron Radiation Facility.*

The ID21 ESRF is beamline dedicated to X-ray and FTIR micro-spectroscopy. Localization and speciation of trace elements is primarily done using micro-X-ray fluorescence ( $\mu$ XRF) and micro X-ray absorption spectroscopy ( $\mu$ -XANES) in the tender X-ray domain (now extended to 2-9.2 keV). ID-21 has sensitivity in the low ppm range and allows localization with a sub-micron beam of various elements. The scanning X-ray microscope (SXM) is designed to cover a relatively wide range of elements of interest in nanotoxicology. The SXM offers a very high versatility in terms of focusing optics, detection and sample environment. The X-ray beam spot size can be tuned from macro (200  $\mu$ m) to sub-micro ( $\sim$ 500 nm), which then allows localization of trace elements at subcellular level. A large panel of complementary detectors is available and provides: high sensitivity, high throughput, or high spectral resolution, which enables the collection of  $\mu$ -XRF and  $\mu$ -XANES spectra on a large variety of biologically relevant samples. The samples can be studied in various conditions (room temperature, cryo, wet cells). In particular, the analysis in cryogenic conditions allow the study of frozen hydrated specimens (cells and cryo-sectioned tissues) preventing elemental redistribution and minimizing radiation damage. Due to the penetration depth of X-rays ultramicrotome sectioning is not required like in transmission electron microscopy and frozen hydrated cells can be studied without sectioning. The X-ray scanning microscope is therefore highly appropriate for in-situ studies of trace metals used in nanotechnology such as Ti, Cr, Fe, Co, Ni, Cd, Ce, Ag and Cu, and gives simultaneously access to mapping and speciation of lighter elements such as P, S, Ca which can be involved in fixation/elimination mechanisms. This combined approach allows studying the chemical modifications of NPs in biological systems down to sub-cellular level. Additionally, ID21 has a SR-based FTIR end-station that can provide complementary molecular mapping, with a  $\sim$ 5 $\mu$ m lateral resolution. In summary, ID21 offers a multimodal set up of state-of-the-art techniques for micro-spectroscopies in life sciences. Results obtained at the beamline in the study of Ti, Ce and Ag nanoparticles will be discussed.

**C6: “Effect of Cd (II) concentrations upon selenium speciation in cauliflower (*Brassica spp.*)”** *Rene Loredó-Portales, Gustavo Cruz-Jiménez, Diana O. Rocha Amador, Minerva Martínez Alfaro, Guadalupe de la Rosa, J. Jorge Delgado, Universidad de Guanajuato. Jorge Gardea-Torresdey, The University of Texas at El Paso.*

Recent studies have shown selenium reduces the toxic effect of some toxic metals. In *Phaseolus vulgaris* this effect is observed when cadmium is added in nutrient solution; however, arsenic enhances its toxicity in selenium presence. Nowadays there is not enough information about the interaction of selenium with other toxic elements in plants. Therefore, this work is focused in the interaction of selenium and cadmium in cauliflower (*Brassica spp.*). The experimental design used for this purpose used three concentrations of Se(IV) and Se(VI) : 0.1, 2 and 5 ppm. Cadmium was added as Cd(II) in 0.1 and 5.0 ppm. Seedlings were grown in a modified Hoagland’s solution during 30 days. After that, the

seedlings were divided in shoot and root parts, lyophilized and triturated. Then the powder obtained was mounted in aluminum folders for XAS analysis. The results shown that selenium reduced Se(IV) and (VI) in selenium-organic forms in both roots and shoots. Selenium reduction could be associated to the low toxic effect showed at the different cadmium concentrations.

**S6: Caracterización de PM10 y especiación de Fe por espectroscopia de absorción de rayos-x para la identificación de la fuente emisora de la ciudad de León, Gto.** Gladys Morales López, Ma. Guadalupe García Jiménez, J. Merced Martínez Rosales, Guadalupe de la Rosa, Gustavo Cruz-Jiménez, Universidad de Guanajuato, México. Marcos Delgado Ríos, Universidad Autónoma de Ciudad Juárez.

Se realizó la caracterización de material particulado PM10, proveniente del monitoreo de un área de la ciudad de León, Gto. Las muestras de PM10 se obtuvieron del muestreo en equipo de alto volumen colectándose 12 muestras durante el período febrero-octubre de 2008. Los elementos analizados fueron As, Cu, Cr, Fe y Pb, la concentración total de estos metales se obtuvo por Espectroscopía de Absorción Atómica. Los resultados muestran que el Fe es el metal que presenta las concentraciones más altas. Debido al impacto potencial a la salud humana del Fe presente en material particulado, se procedió a realizar la especiación del mismo por Espectroscopía de Absorción de Rayos- X. El estado de oxidación del Fe presente en las muestras se obtuvo del análisis de los espectros XANES mediante ajuste de combinación lineal de las muestras con Fe, FeSO<sub>4</sub>, Fe(NO<sub>3</sub>)<sub>3</sub>, Fe<sub>2</sub>(SO<sub>4</sub>)<sub>3</sub>, Fe<sub>2</sub>O<sub>3</sub> y FeCl<sub>3</sub> como compuestos modelo, los resultados muestran que el estado de oxidación es Fe<sup>3+</sup>. Para determinar las especies de Fe, así como la fuente emisora se realizó un análisis de LC-XANES fitting con los compuestos modelo citados y muestras reales de suelo y polvos. El análisis muestra que las posibles especies de Fe son Fe(NO<sub>3</sub>)<sub>3</sub>, Fe<sub>2</sub>(SO<sub>4</sub>)<sub>3</sub> y Fe<sub>2</sub>O<sub>3</sub>; además las fuentes emisoras son suelo debido a la erosión eólica y polvo de resuspensión debida a tráfico vehicular.

**C7: A Dispersive XANES and XRD Investigation of the Reducibility and Crystallization Processes of Iron Oxides Promoted by Gold,** Juan C. Fierro-Gonzalez, Instituto Tecnológico de Celaya, México.

Supported gold catalysts are typically more active for oxidation reactions when the supports are reducible metal oxides (e.g., Fe<sub>2</sub>O<sub>3</sub>, CeO<sub>2</sub>, etc.) than when they are non-reducible metal oxides (e.g.,  $\gamma$ -Al<sub>2</sub>O<sub>3</sub>, MgO, etc.). This observation has led some authors to conclude that redox processes taking place at the gold-support interface might play an important role in the catalysis. H<sub>2</sub>-temperature-programmed reduction (H<sub>2</sub>-TPR) has been used to investigate the influence of gold on the reducibility of transition metal oxide supports. However, for some iron oxide-supported gold samples it has been observed that H<sub>2</sub>-TPR peaks attributed to the reduction of Fe<sup>3+</sup> and Au<sup>3+</sup> overlap, complicating the interpretation of the data. In this work we used dispersive X-ray absorption near edge structure (XANES) at the Au-LIII and Fe-K edges as iron oxide-supported gold samples were treated in flowing H<sub>2</sub> at increasing temperature. We combined the XANES data with X-ray diffraction (XRD) results

and demonstrated that the onset of reduction of Fe<sup>3+</sup> and the crystallization of the support occurred at lower temperature in samples containing gold than in samples of the bare iron oxide. We propose that the reduction process could be promoted by the activation of hydrogen on reduced gold sites.

**C8: High-pressure behavior of the oxygen storage material YBaCo<sub>4</sub>O<sub>7</sub>: A synchrotron X-ray diffraction study.** *E.A. Juarez-Arellano(a), M. Avdeev(b), L. Bayarjargal (c), A. Friedrich (c), B. Winkler (c).* (a) Universidad del Papaloapan, Circuito Central 200, Parque Industrial, 68301 Tuxtpec, Oaxaca, México. (b) Bragg Institute, ANSTO, PMB 1, Menai, NSW 2234, Australia. (c) Institut für Geowissenschaften, Goethe-Universität Frankfurt, Altenhaferallee 1, 60438 Frankfurt A.M., Germany.

Recently, a new family of isostructural cobaltates (M<sub>2</sub>BaCo<sub>4-x</sub>R<sub>x</sub>O<sub>7</sub>, M = In, Y, Ln; R = Co, Fe, Zn) has been synthesized [1]. These cobaltates belong to a new class of geometrically frustrated magnets which not only exhibit interesting magnetic-, electronic-, thermoelectric- and electrochemical properties, but they also have a remarkable low-temperature oxygen absorption/desorption capability which makes them suitable as oxygen sensors, oxygen permeation membranes and solid oxide fuel cells. It has been shown that the oxygen uptake and release process is related to the ability of the cobalt atoms to adopt different oxidation states (Co<sup>2+,3+,4+</sup>), while the geometrically frustrated magnetism is related to the Kagomé layers in their crystal structure [2]. Although these cobaltates have been studied intensively, little was known about the influence of pressure on the crystal structure behavior of this class of compounds [3]. In this presentation, the main characteristics of the cobaltates compounds M<sub>2</sub>BaCo<sub>4-x</sub>R<sub>x</sub>O<sub>7</sub> (M = In, Y, Ln; R = Co, Fe, Zn) will be reviewed. We will show the existence of pressure-induced phase transformations, which are followed by a continuous amorphization process. The high-pressure behavior of this class of materials will be compared to that of isostructural compounds and the influence of the oxygen-content on the overall high-pressure behavior will be discussed. [1] M. Valldor, M. Andersson, *Solid State Sci.* 4 (2002) 923–931. [2] O. Chmaissem, H. Zheng, A. Huq, P. W. Stephens, J. F. Mitchell, *J. Solid State Chem.* 181 (2008) 664–672. [3] E. A. Juarez-Arellano, A. Friedrich, D. J. Wilson, L. Wiehl, W. Morgenroth, M. Winkler, B. Avdeev, R. M. Macquart, C. D. Phys. Rev. B 79 (2009) 064109.

**C9: Synchrotron microtomography under extreme conditions,** *Michelle Alvarez Murga,* European Synchrotron Radiation Facility, EU.

Microtomography is a non-destructive method widely used for reconstructing 3D images from 2D angular projections. It uses X-rays or neutrons to penetrate the matter and access different physical magnitudes (i.e. absorption, diffraction, fluorescence). Combined with synchrotron X-ray beams it provides high spatial-resolutions (μ-nm), and high energies required for the characterization of heavy-elements or samples in complex environments. Applied under extreme conditions (high-pressure-high-temperature and/or deformation) this probe could provide insight in the evolution of microstructure, phase distribution, strain-state and volume changes of materials. It could cover a wide range of potential applications in geology, physics, chemistry and materials science. However,

microtomography studies under high-pressure remain limited to a few examples. The principal cause is that they require the rotation of the sample chamber under load. We present the development of high-pressure microtomography within a new rotating Paris-Edinburgh cell (RoToPEC). Such a non-destructive submicron-probe provides 3D insight of the structure (diffraction) and density (absorption) of crystalline and amorphous phases synthesized in situ under extreme conditions. The ability to rotate 360° the sample chamber, overcomes the sample-access limitation of ordinary high-pressure cells and allows to operate in additional modes such as shearing or deformation. The potential of this experimental technique is demonstrated by in situ studies of: (i) C60 phase transformations, (ii) precise volume measurements  $V(P, T)$  and (iii) deformation of metals. This work is collaboration between beamline ID27 at the ESRF, dedicated to X-ray powder and single crystal diffraction; the Neel Institute in Grenoble, dedicated to the study of matter under extreme conditions; and the Institut de Minéralogie et de Physique des Milieux Condensés in Paris, dedicated to development of high-pressure cells. « New generation of large volume cells for research under extreme conditions» High Pressures network Project CNRS 2009 – MRCT 2010-11 Contact details: Michelle Alvarez [michelle.alvarez@esrf.fr](mailto:michelle.alvarez@esrf.fr), [michelle.alvarez-murga@grenoble.cnrs.fr](mailto:michelle.alvarez-murga@grenoble.cnrs.fr), M.Sc. Materials Science and Engineering PhD Student, Dynamics and Extreme Conditions Group ID27 - High Pressure Beamline European Synchrotron Radiation Facility – ESRF 6 rue Jules Horowitz, B.P. 220, F-38043 Grenoble Cedex, France Tel: +33 (0)4 76 88 23 17 Institut Néel CNRS-UJF Structure et Propriétés des Matériaux – Conditions Extrêmes 25 Avenue des Martyrs, B.P. 166, F-38042 Grenoble Cedex, France Tel: +33 (0)4 76 88 74 2.

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#### FRIDAY JUNE, 8th

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**S7: Radon Exhalation Rate in Soil from Fresnillo City, Zacatecas, México.** *Iris Selene Gomez Quiñones*, Unidad Académica de Estudios Nucleares, Univ. Autónoma de Zacatecas, México.

This investigation work was carried out to locate areas of high radon exhalation at Fresnillo city, Zacatecas, Mexico, since the gas radon symbolizes the radiological risk to the human exhibition and the soil is the main source from generation of this gas. Exhalation measurement at different depths between 25 and 35 cm was realized applying two methods: Open vial and scintillation counting. Exhalation rate in sampled points varied from

**IT4: Pictures of materials: x-ray imaging at the Advanced Photon Source.** *Chris Jacobsen*, Argonne Lab/Northwestern University, USA.

X rays provide a window into the structure of materials, through diffraction and spectroscopy. The addition of imaging to these techniques allows one to uncover details in real-world, heterogeneous materials. Imaging research at the Advanced Photon Source at Argonne Lab is described, including rapid tomography of dynamic materials, ultrafast movies of explosions, and nanoscale 3D imaging of trace elements in cells. Perspectives for the future are then discussed.

**S8: Analytical study of selenium and cadmium in *Lepidium sativum* grown under different exposure conditions.** Eunice Yáñez Barrientos, Julio César Torres Elguera, Kazimierz Wrobel, Katarzyna Wrobel, Universidad de Guanajuato, México.

The present work had been undertaken as a part of larger metallomic study designed to get a deep insight into the fate of Cd and Se and their possible effects in *Lepidium sativum*. This plant is an edible vegetable from Se-accumulating Brassicaceae family and it has often been used for assessing phytotoxicity of contaminated environments 1, 2; however information on its defensive response under exposure to metals/metalloids and on their combined effect is scarce. We had previously shown that cadmium toxicity in garden cress is manifested by growth inhibition, lower status of micronutrients and increased oxidative stress. Similar, but less pronounced phytotoxic effects were observed if only Se(IV) was added to the growth medium. In the cultures simultaneously exposed to Cd(II) and Se(IV) up to 2.0 mg L<sup>-1</sup>, the adverse effect of both elements tended to disappear. In particular, a protective effect of selenium against cadmium toxicity was clearly observed and it was proposed that the beneficial effect of selenium might be due to the direct interaction between two elements<sup>3</sup>. In search of further experimental data confirming such interactions, plants were again grown in the presence of Cd(II), Se(IV), Cd(II) + Se(IV) and the two elements were determined in the whole biomass as well as in three operationally defined fractions (I –soluble, non-protein compounds, II- soluble proteins; III- insoluble proteins, polysaccharides, lipids and sub-cellular structures). Additionally, fraction II was analyzed by SEC-ICP-MS (78Se y 111Cd). The results obtained showed significantly lower uptake of Cd and Se in plants exposed to their mixtures as compared to those grown in the presence of a sole element. Furthermore, when the growth medium contained Se(IV) + Cd(II), the relative distribution of the two elements was different in fraction I (lower) and in fraction III (higher) with respect to the individually exposed plants. The results obtained by SEC-ICP-MS in fraction II suggest that the second element (Se(IV) + Cd(II)) might affect the incorporation of Cd and Se to the high and medium MM compounds. Overall, these results confirm the interaction of Cd and Se forms in vivo, however analytical speciation is needed for identification of chemical species involved. (1) Latif, M.; Licek, E. *Environ Toxicol* 2004, 19, 302-309. (2) Oleszczuk, P. *Environ Toxicol* 2010, 25, 38-47. (3) Yanez Barrientos, E.; Rodriguez Flores, C.; Wrobel, K.; Wrobel, K. *J Mex Chem Soc* 2012, 56, 1-7.

**S9: Mechanisms of interaction with hexavalent chromium of the environmental strain Ed8 of *Aspergillus niger* var. *Tubingensis*,** A. Lopez Torres (1), Félix Gutiérrez Corona (1), P.L. Rodriguez Carrillo(1), V.B. De León Rodríguez (1), A.R. Corrales Escobosa (1), G. Cruz Jiménez (2), G. de la Rosa Álvarez (3). (1) Departamento de Biología, División de Ciencias Naturales y Exactas, Universidad de Guanajuato, Campus Guanajuato.(2) Departamento de Farmacia, División de Ciencias Naturales y Exactas, Universidad de Guanajuato, Campus Guanajuato. (3) Departamento de Ingeniería Química Electrónica y Biomédica, División de Ciencias e Ingenierías, Universidad de Guanajuato, Campus León.

Chromium compounds may occur as environmental contaminants present in ground waters, soils and industrial effluents due to their extensive use in various industries. Chromium uptake by the biomass of strain Ed8 of *A. niger* var. *tubingensis*, a chromate-tolerant fungal strain previously isolated from a chromium-polluted soil, was studied in shake flask cultures, in minimal medium of pH 5.3 containing 0.17 mM potassium dichromate and amended with

different sulfur sources, either methionine (0.268 mM), or sulfate in low (0.416 mM) or high (31 mM) concentration. It was observed that in medium with low concentration of sulfate strain Ed8 biomass can incorporate about 5.5 times more chromium with respect to the biomass incubated in medium with high concentration of sulfate, while in medium with methionine as a sulfur source the biomass is able to incorporate 3 times more chromium with respect to the culture medium with high concentrations of sulfate. The decrease in Cr(VI) levels in the culture supernatant was about 85% in medium with high concentration of sulfate and with methionine, while in medium with low concentration of sulfate such decrease was about 10%. X-ray absorption spectroscopy (XAS) is a proven technique used to elucidate the oxidation state of different elements in solid, liquid and aqueous sample. This technique was used to determine the presence of Cr(VI) and Cr(III) in the supernatant from cultures incubated with high sulfate concentration, as well as in the biomass obtained from cultures grown in medium with methionine or with low sulfate concentration. XANES spectra was obtained using the chromium K-edge (5989 eV) as calibration energy for samples and model compounds. The characteristic Cr(VI) pre-edge was used to determine its presence in samples. Spectra XANES analysis indicated that Cr(III) formed in the extracellular space and in the intracellular environment is mainly associated to the phosphate chemical form. These results indicated that the transformation of Cr(VI) to Cr(III) occurred both in the extracellular medium and in the biomass of Ed8 strain; these findings point to the usefulness of XANES technology to determine the subcellular distribution of chromium species and their chemical environment.

**C10: “ X- ray Absorption Spectroscopy used for element speciation in environmental samples”** *Gustavo Cruz-Jiménez*, Universidad de Guanajuato.

X-ray Absorption Spectroscopy (XAS) is an innovative technique used to analyze the oxidation states and the chemical environment of different toxic elements in the environment. The chemical information obtained through this technique allows scientists to determine the toxicity and mobility of several elements in the environment. XAS allows to determine the local coordination environment of elements in crystalline and amorphous solids, liquids, and aqueous samples. In this technique, some samples do not require chemical pretreatment, therefore chemical speciation is more reliable than other techniques. In addition, it is a non-destructive technique and it requires a minimum quantity of sample (in the order of milligrams). This work shows an overview of the application of this technique in environmental samples. Speciation of Se, Cu, Cr, S, As, Pb, Br and Fe is presented in different environmental materials such as soils, plants, mine tailings and air particulates.

**S10: Image generation in EDXRF spectroscopy**, *Gilberto Gutiérrez-Vázquez*, Universidad de Guanajuato.

A prototype for scanning and imaging of solid samples using EDXRF technique is presented. Hardware and software were original and fully developed in a LabView environment. This experimental research can be useful for rapid evaluation of samples to be processed in synchrotron type studies.

**S10: Undulator Radiation inside a Dielectric Waveguide.** *Anna Kotanjyan*, Yerevan State University, Armenia.

We investigate the radiation from a charge moving along a helix around a dielectric cylinder immersed in a homogeneous medium. The radiation intensity in the exterior medium at large distances from the cylinder has been considered previously and here we are mainly concerned with the radiation propagating inside the cylinder. The expressions for the bound modes of the radiation field are derived in both interior and exterior regions. The radiation intensity for the modes propagating inside the cylinder is evaluated by using two different ways: by evaluating the work done by the radiation field on the charge and by evaluating the energy flux through the cross-section of the cylinder. The relation between these two quantities is discussed. We investigate the relative contributions of the bound modes and the modes propagating at large distances from the cylinder to the total radiation intensity. Numerical examples are given for a dielectric cylinder in the vacuum. It is shown that the presence of the cylinder can lead to the considerable increase of the radiation intensity. The insertion of a dielectric waveguide provides an additional mechanism for tuning the characteristics of the undulator radiation by choosing the parameters of the waveguide. The radiated energy inside the cylinder is redistributed among the cylinder modes and, as a result, the corresponding spectrum differs significantly from the homogeneous medium or free-space results. This change is of special interest in the low-frequency range where the distribution of the radiation energy among small number of modes leads to the enhancement of the spectral density for the radiation intensity. The radiation emitted on the waveguide modes propagates inside the cylinder and the waveguide serves as a natural collector for the radiation.

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