



14th SESAME Users Meeting

3rd – 4th December, 2016
Days Inn Hotel, Amman, Jordan

Scientific Program

1st Day: Saturday, December 3rd, 2016

08:30 – 9:30	Registration & Poster Hanging
9:30 – 10:00	Welcome and Opening Session
10:00 – 10:30	Coffee Break + Group Photo
10:30 – 10:50	“Recent Developments of the SESAME Accelerator Complex” Erhard Huttel
10:50 – 11:10	“Scientific Program Perspectives of SESAME” Giorgio Paolucci
11:10 – 11:30	“Towards User Access to SESAME: the SESAME User Committee (SUC)” Özgül Öztürk
11:30-12:00	“The Open SESAME EU project: an Opportunity for SESAME and its User Community” Edward Mitchell
12:00-12:30	"A New Twist of the Solid-State Chemistry: Dynamic Molecular Crystals" Pance Naumov
12:30 – 13:00	“The Virtual Research Environment: Vi-SEEM Project” Salman Matalgah
13:00 – 13:45	Lunch Break + Poster Session (Hosted by: JAEC)
14:00-15:00	Practical sessions (1, 2) [Session's duration is 30 minutes each] (1): “Proposal writing and Access: Science and methodology” SESAME User Committee (SUC) (2): “Demonstration of SESAME Users’ Office” Giorgio Paolucci
15:10	Departure to SESAME Site (Vouchers at the Registration Desk) <i>* For the visit to SESAME, service buses will be waiting at the entrance of the “Days Inn” hotel. The buses will depart to SESAME site at 15:10 pm. Please, make sure to be present in front of the hotel entrance at least 5 minutes before the departure time. ACCESS TO BUSES WILL BE STRICTLY ALLOWED TO VOUCHERS’ HOLDERS.</i>
16:00 – 17:00	SESAME Site Tour

17:15	Departure to Amman
20:00 – 21:30	Dinner

2nd Day

Sunday, December 4th, 2016

08:30 – 09:10	“Science at Elettra and FERMI” (provisional) <i>Maya Kiskinova (Invited)</i>
09:10-09:50	“Infrared beamlines at Synchrotron Facilities: Worldwide Status, Present and Challenging Perspectives ” <i>Paul Dumas (Invited)</i>
09:50-10:10	“FIR (THz) spectroscopy of semiconductor based Low dimensional electronic systems” <i>Mehdi Pakmehr</i>
10:10 – 10:30	Coffee Break + Posters' Session
10:30-11:10	“Efforts towards 1st protein crystal structure determination in Pakistan with recent updates” <i>Muhammad Imran (Invited)</i>
11:10-11:40	“PILATUS 300K for SESAME's Material Science Beamline” <i>Dubravka Jung (Invited)</i>
11:40-12:00	“Novel graphene-titania interfaces as a potential catalytic material towards clean energy production” <i>Naila Jabeen</i>
12:00-13:00	Lunch Break + Poster Session
13:00-15:00	Thematic Parallel Workshops (A & B)
15:00	Closing Session and Best Poster Award

2nd DaySunday, December 4th, 2016

Parallel Thematic Workshops (A & B)

(A): Synchrotron Radiation and Life Sciences		
13:00 – 13:30	“Current Status and Progress of SESAME Infrared Beamline”	G. Kamel
13:30- 13:45	“Benign and Malignant Human Breast Tissues Diagnosis: IR-Micro spectroscopic Approach”	S. Rehman
13:45-14:00	“Dielectric Spectroscopy Measurements on Collagen Blends”	A. Refaat
14:00- 14:15	“Study of Historical Parchments by FTIR & XRD Techniques”	M. Darzi
14:15-14:30	“Mapping of Ancient Teeth Using Vibrational Spectroscopy FTIR and Raman”	W. Sekhaneh
14:30-14:45	“Vi-SEEM Concept and Tutorials”	M. Al-fraheed
14:45-15:00	“Structural Studies on Z. Mobilis Levansucrase”	B. Bakar

(B): Synchrotron Radiation for Environment and Energy		
13:00 – 13:30	“SESAME Materials Science Beamline”	M. Harfouche and M. Abdellatief*
13:30- 14:00	“Beamlines Optical Systems and Ray Tracing”	H. Khosroabadi
14:00- 14:15	“Crystal and Electronic Structure Properties of the Sm _x Fe _{1-x} BO ₃ Oxides”	O. Ozkendir
14:15-14:30	“Local Structure and Cation Distribution in CoLa _{0.15} Fe _{1.85} O ₄ as a Function of the Synthesis Method Determined by X-ray Absorption Spectroscopy”	N. Imam
14:30-14:45	“EXAFS Studies of Nanostructured Finemet-type Alloys”	Y. Swilem
14:45-15:00	“Synchrotron Based Photoemission Studies of (Ga, Mn)As”	I. Ulfat



Oral Presentations

Parallel Thematic Workshops A & B

2nd Day

Sunday, December 4th, 2016

Session A

Synchrotron Radiation and Life Sciences

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“Current Status and Progress of SESAME Infrared Beamline”

GIHAN KAMEL

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ABSTRACT

FTIR Microspectroscopy proved to be a potent technique in life sciences, materials science, cultural heritage, environment, high pressure physics and many others. In this context, and as expressed by letters of interests, the selection and approval to build an Infrared Microspectroscopy beamline at SESAME was recognized, and accordingly was scheduled as a “Day-1” beamline. The main focus is to allow Synchrotron Radiation Infrared Microspectroscopy and imaging, with a reliable capacity to address the diverse requirements of the scientific community.

The talk will focus on the SESAME Infrared beamline design; being the first completely new designed beamline at the facility. I will also explain what has been done so far, what we are currently working on, and what we promise to deliver to the Infrared research groups in the Middle East and beyond.

“Benign and Malignant Human Breast Tissues Diagnosis: IR-Micro Spectroscopic Approach”

SOHAILA REHMAN

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ABSTRACT

FTIR micro spectroscopy technique was used to detect subtle, cancer related alterations in the biochemical and morphological composition of tissues at the microscopic level in order to identify appropriate common biomarkers. Approximately seventy breast biopsy and mastectomy tissues were collected from tertiary hospitals of Islamabad, Pakistan with the proper consent of patient and fulfilled the ethical review protocols. Nine different conditions including Grade -1 to G-111 invasive ductal carcinoma tissues, as well as, normal tissues, were considered for measurements. Complete history of patients gone through mastectomy was entered in data base, Thermo. The formalin-fixed and paraffin-embedded blockswere obtained from pathology laboratory and a ribbon of 8 μm section was trimmed with microtome and placed in water bath (35-40 $^{\circ}\text{C}$) before being deposited on the Low-e-Microscope slides (MirrIR) at 60 $^{\circ}\text{C}$. Nicolet Continuum, IR microscope along with 8700 Thermo Scientific FTIR spectrometer was used for the Infrared micro-spectroscopic experiments at SESAME. The Spectra were acquired in reflection mode with the IR Globar source. Software packages, Thermo OMNIC for spectral acquisition with data processing and The Unscrambler X for multivariate data analysis and design of experiments will be used. Spectral maps of Normal and malignant tissues are systematically analysed to identify the possible biomarkers of the disease.

Key Words: Breast biopsy tissues, Invasive ductal carcinoma, IR-microscopy.

“Dielectric Spectroscopy Measurements on Collagen Blends”

AHMED REFAAT

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ABSTRACT

Molecular modeling at PM6 level for Collagen/Chitosan blend was introduced and showed that blending caused an increase in the total dipole moment indicating increased reactivity. The theoretical results were approved experimentally through carrying out some dielectric parameters, and AC and DC conductivities for some Collagen blends with different ratios. Collagen is blended with other biopolymers to enhance its physicochemical properties for tissue engineering applications. In this study, Collagen was blended with Chitosan at the ratios 30:70, 40:60, 50:50 and 60:40 respectively and with Agarose at the ratios 40:60, 50:50, 60:40 and 70:30 respectively. The measurements of the dielectric constant (ϵ') and the dielectric loss factor (ϵ'') for the blends as well as their AC conductivity (σ_{ac}) and DC conductivity (σ_{dc}) were measured over the frequency range of 100 Hz–5 MHz at room temperature. The conductivity showed steady increase with increasing frequency for both blends. ϵ' for the different ratios of the two blends increased with frequency while ϵ'' for the Collagen/Chitosan blends showed no significant change with increasing frequency with only some decrease at low frequencies. The 70%-30% and 60%-40% Collagen/Agarose blends showed no significant change in ϵ'' with increasing frequency while the 40%-60% and 50%-50% blends showed remarkable increase in ϵ'' at high frequencies.

Keywords: Molecular modeling, PM6, Dielectric constant, Collagen blends, Chitosan, Agarose, conductivity, dielectric loss.

“Study of Historical Parchments by FTIR & XRD Techniques”

MAEDEH DARZI

Maedeh Darzi, Mohammad Lamahi Racht

Isfahan University of Technology

ABSTRACT

Writing materials are comprised of a great variety of media. With the development of human civilization over long periods of time, these media have changed from clay and pottery to the following three most common ones: parchment, papyrus and paper. Among these, parchment (protein-based) has fundamental significance since it has relatively high durability (compared to papyrus and paper (cellulose-based)) and better geographical availability (compared to papyrus). Maintaining the historical, cultural, or figurative messages on these media is possible only if the media do not degrade with time. Thus, studies of composition, structure, morphology and physical-chemical properties of these media are essential components of research in this field. We report here on the use of synchrotron radiation (SR) to satisfy our scientific curiosity and to better understand the process and technology involved in the creation of these media and their degradation over time. In particular, we report on results of studies of parchment fragments using synchrotron Fourier Transform Infrared, Attenuated total reflection- Fourier Transform Infrared (ATR-FTIR) & synchrotron x-ray Diffraction (SR-XRD).

“Mapping of Ancient Teeth Using Vibrational Spectroscopy FTIR and Raman”

WASSEF SEKHANEH

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ABSTRACT

Archaeological bone is an important archaeological witness as it records significant information about past societies. The morphological and structural changes in addition to the chemical composition of archaeological bone material exhibit vital information about bone at different stages of the human development. In this study, Fourier transform infrared (FTIR) spectroscopy and Fourier Transform Infrared Imaging (FTIRI) in addition to Raman spectroscopy and Raman imaging analyses were applied to 16 primary and permanent human teeth samples taken from a Roman archaeological site in Northern Jordan. The samples were examined for their mineral-to-matrix and carbonate to phosphate contents (at 1415 cm⁻¹ and at 1030 cm⁻¹ respectively). The results confirmed the differences in mineral ratios and also carbonate substitution between primary and permanent archaeological tooth samples.

Key words: Ancient bone; Fourier transform infrared spectroscopy; Raman; imaging.

“VI-SEEM: Concept and Training. Case Study: The Cancer Cell Classification”

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ABSTRACT

Recently, several efforts have been introduced in context of life science; Medical Image Applications, Historical image Processing and ... etc. One of the medical image applications concerns of the cancer disease. This kind of application depends on using the computerized analysis for the cancer cells. The latter are processed to be presented into different electronic shapes (e.g. digital Microscopy Images, Mammogram Images and ... etc. The computerized analysis, in turn, is required not only to process the data of the cancer cells but also to classify automatically the negative and positive cancer data. In this work, an application is introduced to be developed for cancer cells classification. The first process of the proposed application is the automatic segmentation in which a threshold value is automatically determined. In addition, the texture features have to be automatically extracted. The second process includes using the machine learning algorithms (i.e. genetic algorithm, AdaBoost Algorithm, Fuzzy Logic and Neural Network) for supporting the computerized analysis and classification tasks. OpenCV and MatLab software are used to develop the proposed application. The results will be published for public domain in cooperation with the project VI-SEEM.

“Structural Studies on *Z. Mobilis* Levansucrase”

BAHAR BAKAR

Bahar Bakar, Burcu Kaplan Türköz

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ABSTRACT

Levansucrases (Lsc) are enzymes, which have both sucrose hydrolysis and transfructosylation activity. Depending on the fructosyl acceptor, levansucrase will produce different products like levan and fructooligosaccharides (1). *Zymomonas mobilis* levansucrase (ZmLsc) can produce both FOS and levan depending on the reaction parameters, such as temperature and initial substrate concentration (2). Levan is a fructose homopolymer, with anti-inflammatory, anti-oxidant and anti-bacterial properties (3). FOS are low calorie sugars which are fermented by bifidobacteria, so they can be used as prebiotics. (4). Thus, the understanding of control mechanism of the selective production of these biologically important fructans is important. Our current studies are focused on purification of the enzyme in order to solve its atomic structure using macromolecular crystallography. In parallel to experimental studies, we are also using structural bioinformatics for modeling the structure of ZmLsc and comparing its structural details with other microbial levansucrases.

Keywords: Levansucrase, *Zymomonas mobilis*, Crystallization, structural bioinformatics

References:

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2. Santos-Moriano, P., 2015. Journal of Molecular Catalysis B: Enzymatic, 119, 18–25.
3. Öner ET, et al., 2016. Biotechnol Adv 34: 827–844.
4. Sabater-Molina M, et al., 2009. J Physiol Biochem 65: 315–328.

Acknowledgements: This work is supported by TÜBİTAK-TOVAG (grant number:214O174).

Session B

Synchrotron Radiation for Environment and Energy

(B): Synchrotron Radiation for Environment and Energy		
13:00 – 13:30	“SESAME Materials Science Beamline”	<i>M. Harfouche and M. Abdellatief*</i>
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14:15-14:30	“Local Structure and Cation Distribution in CoLa _{0.15} Fe _{1.85} O ₄ as a Function of the Synthesis Method Determined by X-ray Absorption Spectroscopy”	<i>N. Imam</i>
14:30-14:45	“EXAFS Studies of Nanostructured Finemet-type Alloys”	<i>Y. Swilem</i>
14:45-15:00	“Synchrotron Based Photoemission Studies of (Ga, Mn)As”	<i>I. Ulfat</i>

“SESAME Materials Science Beamlines”

MAHMOUD ABDELLATIEF

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ABSTRACT

The SESAME Materials Science MS beamline for X-ray diffraction XRD applications, is presently under construction in Allan, Jordan. The beamline is based on components previously installed at the Swiss Light Source, but modifications in the beamline design have been introduced to match the characteristics of the SESAME storage ring. The SESAME MS beamline will accommodate XRD experiments in the energy range between 5 and 25 keV. The beamline ray tracing analysis at 10 keV estimates the flux at the sample to be in the order of 10¹³ (photons/s), the energy resolution is about 2 eV and the effective beam size at the sample of 300 x 2800 μm^2 . Investigations of microstructure will be possible as the instrumental broadening, resulted from simulating the diffraction pattern for a standard material, is in the order of 0.01 $\circ$ at 15 keV. A wide range of applications will be possible at the beamline, such as powder diffraction studies, single crystals and in-situ XRD. The commissioning of the beamline is expected to be in the second half of 2017.

“Beamlines Optical Systems and Ray Tracing”

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ABSTRACT

In this talk, the role of the optical systems in the synchrotron beamlines will be described. Then the ray-tracing simulation method for design and optimization of the beamline will be discussed. The results of ray tracing simulation of the SESAME Material Science beamline by Shadow3 and using new Oasys interface will be presented as a case study.

“Crystal and Electronic Structure Properties of the $\text{Sm}_x\text{Fe}_{1-x}\text{BO}_3$ Oxides”

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ABSTRACT

Influences of Samarium substitution in the Ferric Borate oxide materials were investigated on their crystal, electric and electronic properties. Studies mainly carried on the change in the crystal structure with the increasing Sm substitutions with the collected data from the synchrotron facilities. All prepared samples were determined as semiconductors with weak antiferromagnetic (AFM) ordering at the room temperatures. The main technique for the investigations was X-ray absorption near-edge spectroscopy (XANES) and the collected data were used to probe in the electronic structure properties of the samples. Prominent changes and phase transitions in the crystal structure were observed according to the increasing Sm substitutions. Besides, iron atoms and their 3d levels were determined as the center of the interplays during the entire crystallographic phenomena.

Keywords: Absorption spectroscopy; Electronic structure; Crystal Properties; Oxides

“Local Structure and cation Distribution in CoLa_{0.15}Fe_{1.85}O₄ as a Function of the Synthesis Method Determined by X-ray Absorption Spectroscopy.”

NEAMA IMAM

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ABSTRACT

We have characterized the structure of nanosized La³⁺ substituted CoFe₂O₄ spinel ferrite of composition CoLa_{0.15}Fe_{1.85}O₄ combining x-ray diffraction (XRD) and x-ray absorption spectroscopy (XAS). We analyzed and compared three products from different synthesis routes: (a) standard ceramic technique, (b) citric acid (citrate) and (c) urea assisted flash auto-combustion process. XRD was used to determine the average structure to be used as structural model for the extended x-ray absorption fine structure EXAFS data analysis. The latter has been done using a multi-edge approach by measuring the K edges of Fe and Co and the La L₃-edge. By using the two techniques we determined the cation distribution over the two spinel sublattices (tetrahedral and octahedral). It was found that, the inversion parameter, cation distribution, and the local structure depend strongly on the synthesis routes which in turn influence the La³⁺ lattice-site and vacancies. In addition, the oxidation states of Fe, Co, and La cations were determined by x-ray absorption near edge structure (XANES).

Keywords: XANES; EXAFS; XRD; CoLa_{0.15}Fe_{1.85}O₄; Local Structure; Cation distribution; Inversion parameter.

“EXAFS Studies of Nanostructured Finemet-type Alloys”

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ABSTRACT

The nanostructure of a nanocrystalline Fe₆₆Cr₈Cu₁Nb₃Si₁₃B₉ alloy has been studied by synchrotron radiation extended X-ray absorption fine structure (EXAFS) and analyzed by the cumulant method. Application of the cumulant method enables us to determine the nearest-neighbor interatomic distance and the coordination number for chromium and copper atoms, and thus we are able to obtain detailed knowledge about the role of both Cr and Cu in the structure of nanocrystals at various stages of crystallization. A detailed analysis of the distribution of alloying elements in the grains and grain boundaries reveals the accumulation of Cr in the surrounding of Fe(Si) nanocrystals. The presence of Cr in the surroundings of Fe(Si) can influence the content's arrangement of the nanograins, allowing diffusion of Si atoms in the grain boundaries. Simulated X-ray absorption spectra of the model produced by FEFF9.05 and the proposed Cu clustering of 19 atoms with average cluster size of about 0.4 nm show a good resemblance to the experimental data of the Cu k-edge.

“Synchrotron Based Photoemission Studies of (Ga,Mn)As”

INTIKHAB ULFAT

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ABSTRACT

Magnetic semiconductors combine magnetism and controllable charge transport which are the key features needed in information technology and are thus considered as the potential device material for future spintronics. Nevertheless, there is still no material produced that could be used in common devices. One of the main hurdles is the low temperature that is needed for the ferromagnetic state: (Ga,Mn)As, the material with the highest transition temperature to the ferromagnetic state, still requires cooling to around 200 K. As the basic principles about the mechanisms underlying ferromagnetism in (Ga,Mn)As are still under debate, there is an obvious need for detailed experimental information that can provide important clues towards an improved understanding. Having access to a dedicated MBE system directly connected to a high-resolution photoelectron spectrometer at the synchrotron radiation laboratory MAX-lab, we present a summary of our synchrotron-based spectroscopic investigations of (Ga,Mn)As to reveal the electronic structure of the material.