

Meeting in the framework of the Joint Research Project of  
“Particular Relevance” Serbia – Italy

*‘Nanoscale Insights in Radiation Damage’*

Ministero degli Affari Esteri (MAE)

Thursday, 18 september 2014  
Biblioteca ISM

## Program

- 10:15 – 10:30 Dr. Lorenzo Avaldi, CNR-ISM, Italian Coordinator  
*Opening*
- 10:30 – 11:15 Dr. Daniele Catone, CNR-ISM  
*‘Mass Spectrometry and Synchrotron radiation. Activity and Perspective on CiPo Beamline.’*
- 11:15 – 12:00 Dr. Aleksandar Milosavljevic, Institute of Physics, Belgrade  
*‘VUV and soft X-ray action spectroscopy of biopolymers stored in a linear ion trap’*
- 12-14 Lunch
- 14:00 – 14:45 Dr. Pietro Calandra, CNR-ISMN  
*‘Is electrospray emission really due to net charges?’*
- 14:45 – 15:30 Dr. Stefano Turchini, CNR-ISM  
*‘Soft landing: from small molecules to proteins’*
- 15:30 – 16:00 Dr. Lorenzo Avaldi, Italian Coordinator  
*Discussion and concluding remarks*





# AVVISO DI SEMINARIO



Giovedì 18 Settembre 2014

*Biblioteca dell'Istituto di Struttura della Materia*

**Dr. Daniele Catone**

*CNR - Istituto di Struttura della Materia*

## ***MASS SPECTROMETRY AND SYNCHROTRON RADIATION. ACTIVITY AND PERSPECTIVE ON CiPo BEAMLINE.***

The use of synchrotron radiation in the VUV range coupled with mass spectrometry gives the possibility to perform measurements in single photon regime and most important grants, with its broad tenability, the possibility to acquire photoionization and photofragmentation efficiency curves of selected ions and fragments in a wide energy range, overwhelming the limit of the laser that cannot generate a continuous VUV energy spectrum. In this way the fragmentation processes and the chemical reactivity of molecular and clustered systems can be correlated with the electronic properties of their valence and core states.

The lecture will describe the experimental activity at the Circular Polarization (CiPo) Beamline in the field of photoionization mass spectrometry and photoinduced ion chemistry. Moreover, the perspective of a new experimental apparatus for the photofragmentation of large biomolecules produced in gas phase by ESI will be presented.



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**Dr. Aleksandar Milosavljević**  
*Institute of Physics, Belgrade, Serbia*

## **VUV AND SOFT X-RAY ACTION SPECTROSCOPY OF BIOPOLYMERS STORED IN A LINEAR ION TRAP**

A novel experimental technique that allows vacuum-ultraviolet (VUV) and soft X-ray action spectroscopy of biopolymers stored in a linear ion trap will be presented. The technique is based on tandem mass spectrometry of electrosprayed ions, activated by VUV and soft X-ray synchrotron radiation. The photon activation of trapped precursor ions has been performed by coupling a commercial linear quadrupole ion trap (Thermo scientific LTQ XL), equipped with the electrosprayed ions source, to a synchrotron beamline (SOLEIL, France) [1,2]. The lecture will include a description of the experimental setup and the method, a short review of recent investigations on structure and charge-state dependence of the gas-phase ionization energy of proteins [3], nanosolvation-induced stabilization of fragile biomolecular complexes isolated in the gas phase [4,5], gas-phase protein inner-shell spectroscopy [6] and tandem mass spectrometry of proteins and noncovalent protein-ligand complexes [7].

- [1] A.R. Milosavljević, C. Nicolas et al. J. Synchrotron Rad. 19, 174 (2012)
- [2] A. R. Milosavljević, C. Nicolas et al. Phys. Chem. Chem. Phys. 13, 15432 (2011)
- [3] A. Giuliani, A. R. Milosavljević et al. Angew. Chem. Int. Ed. 51, 9552 (2012)
- [4] A. R. Milosavljević, V. Z. Cerovski et al Angew. Chem. Int. Ed. 52, 7286 (2013)
- [5] A. R. Milosavljević et al, J. Phys. Chem. Letters 5, 1994 (2014)
- [6] A. R. Milosavljević, F. Canon et al. J. Phys. Chem. Letters 3, 1191 (2012)
- [7] F. Canon, A. R. Milosavljević et al., Angew. Chem. Int. Ed. 52, 8377 (2013)



# AVVISO DI SEMINARIO



Giovedì 18 Settembre 2014

*Biblioteca dell'Istituto di Struttura della Materia*

Dr. Pietro Calandra<sup>1</sup>, Francesco Aliotta<sup>2,\*</sup>,  
Mikolaj Pochylski<sup>3</sup>, Rosina C. Ponterio<sup>2</sup>,  
Gabriele Salvato<sup>2</sup>, Cirino Vasi<sup>2</sup>

<sup>1</sup> *CNR-Istituto per lo Studio dei Materiali Nanostrutturati*

<sup>2</sup> *CNR-Istituto per i Processi Chimico-Fisici*

<sup>3</sup> *Adam Mickiewicz University, Poland*

## ***IS ELECTROSPRAY EMISSION REALLY DUE TO NET CHARGES?***

Electrospray ionization (ESI) is a widely adopted soft ionization method for mass spectroscopy (MS). The common belief is that the formation of gas-phase ions takes place at the apex of the Taylor cone via electrophoretic charging. The charge balance would imply that a conversion of electrons to ions should occur at the metal-liquid interface of the injector needle. We have detected that the above description is not consistent with the correct evaluation of the problem [1]. The comparison between experiments performed under the usual geometry and observations obtained under symmetric field configurations suggests that the emitted droplets cannot be significantly charged or, at least, that the presence of charge is not necessary for electrospray jet emission.

[1] J. D. Jackson, Classical electrodynamics, Ch. 4, p 165-168, third edition (John Wiley & Sons, 1999)



# AVVISO DI SEMINARIO



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**Dr. Stefano Turchini**

*CNR - Istituto di Struttura della Materia*

***SOFT LANDING:  
FROM SMALL MOLECULES TO PROTEINS***

The aim of the talk is to present a project for potential applications of ElectroSpray Ionization (ESI) in the nanotechnology. To combine thin films deposition techniques in ultra high vacuum to the controlled deposition of nonvolatile molecules and clusters is of crucial importance. Nowadays applications of ESI in molecule deposition are hampered by the low flux of the ion current. The deposition of a molecular monolayer should not exceed the duration of an hour. A project to design a high flux ESI source to increase the available target density will be presented. The major losses in ion flux occur at pressure in the range 0.1 - 10 Torr, where ion optics is not efficient. Ion funnels are capable of efficiently focusing ions at higher pressures and represent an ideal solution to transmit ions into the mass spectrometer analyzer. In the interaction ion – surface a key role is played by ion kinetic energy, which is a tunable parameter. In the range 1 -100 eV a non-destructive collision between ions and surface can occur with the consequent adsorption/chemisorption of the molecule. Competing processes are surface induced dissociation and elastic scattering.