SATELLITE WORKSHOP - Photon Science

**Present and future opportunities for the investigation of gas-phase biomolecules at FEL and SR facilities**

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| Tue. 24.01.2023 |  |
| Over the past decade, the combination of electrospray ionization sources (ESI), tandem mass-spectrometry (MS) and advanced light sources has become an increasingly popular experimental method for the study of large biomolecules such as peptides, proteins and oligonucleotides. Thanks to the versatility of ESI-MS instruments and the tunability of synchrotrons and FELs in the VUV to X-ray range, our community has collected rich data on e.g. radiation damage, site-selective dissociation, the effects of nano-solvation, spectroscopy of the electronic structure (valence to core levels), insights into geometrical structure, etc. Nevertheless, some experimental challenges are still to be tackled to get deeper knowledge into the studied systems and to be able to record the dynamics of ultrafast processes, photoelectron spectra or to enable coincident/covariance measurements as routinely performed for neutral gas-phase target molecules. With this meeting, we hope to bring together researchers and beamline scientists to discuss ongoing research topics, users’ needs and current possibilities and development at FEL and synchrotron facilities, with a focus on “large” gas-phase biomolecules produced by electrospray ionization. The meeting will end with a round table discussion between users and beamline scientists to stimulate new collaborative projects. | |

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| Organizers: Sadia Bari, Lucas Schwob (DESY) | Contact: sadia.bari@desy.de |

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| **PROGRAMME** | | |
| 09:00 | Welcome and Introduction | Sadia Bari / Lucas Schwob |
| 09:10 | Structural dynamics within gas phase biomolecules upon X-ray, UV and IR photoabsorption: towards probing weak non-covalent bonds relevant in protein folding | Bart Oostenrijk |
| 09:35 | X-ray induced fragmentation of Protonated Cystine | Rebecka Lindblad |
| 10:00 | Soft X-ray spectroscopy studies of gas-phase DNA | Thomas Schlathölter |
| **10:25** | ***Coffee break (20 Min.)*** |  |
| 11:00 | VUV and soft X-rays action spectroscopy of solvated peptides | Alexandre Giuliani |
| 11:25 | The ‘smart’ decomposition of cyclic dipeptides as ‘seeds of life’ | Paola Bolognesi |
| 11:50 | Peptide Bond Formation in Serine clusters following Photon-Induced excitation | Ori Licht |
| 14:00 | The Ion Trap station at BESSY II: Soft X-ray absorption spectroscopy of electrosprayed cations | Vicente Zamudio Bayer |
| 14:25 | TRISS - A new end station in preparation for trapped ion spectroscopy at MAX IV | Noelle Walsch (tbc) |
| 14:50 | Development of the on-the-fly photoelectron spectroscopy of size-selected biopolymer ions at SOLEIL synchrotron | Aleksandar R. Milosavljević |
| 15:15 | The high flux, high stability soft x-ray beamline P04 at PETRA III | Moritz Hoesch |
| 15:40 | Coffee break |  |
| 16:10 | Ultrafast electron dynamics in bio-chemically relevant molecules | Fransceca Callegari |
| 16:35 | FLASH 2020+ - new opportunities for biomolecular research | Markus Gühr |
| 17:00 | MS SPIDOC: Coherent Diffractive Imaging of proteins and viral capsids | Thomas Kierspel |
| 17:25 | Round table discussions | Sadia Bari / Lucas Schwob |
| **18:00** | **End of Meeting** | |