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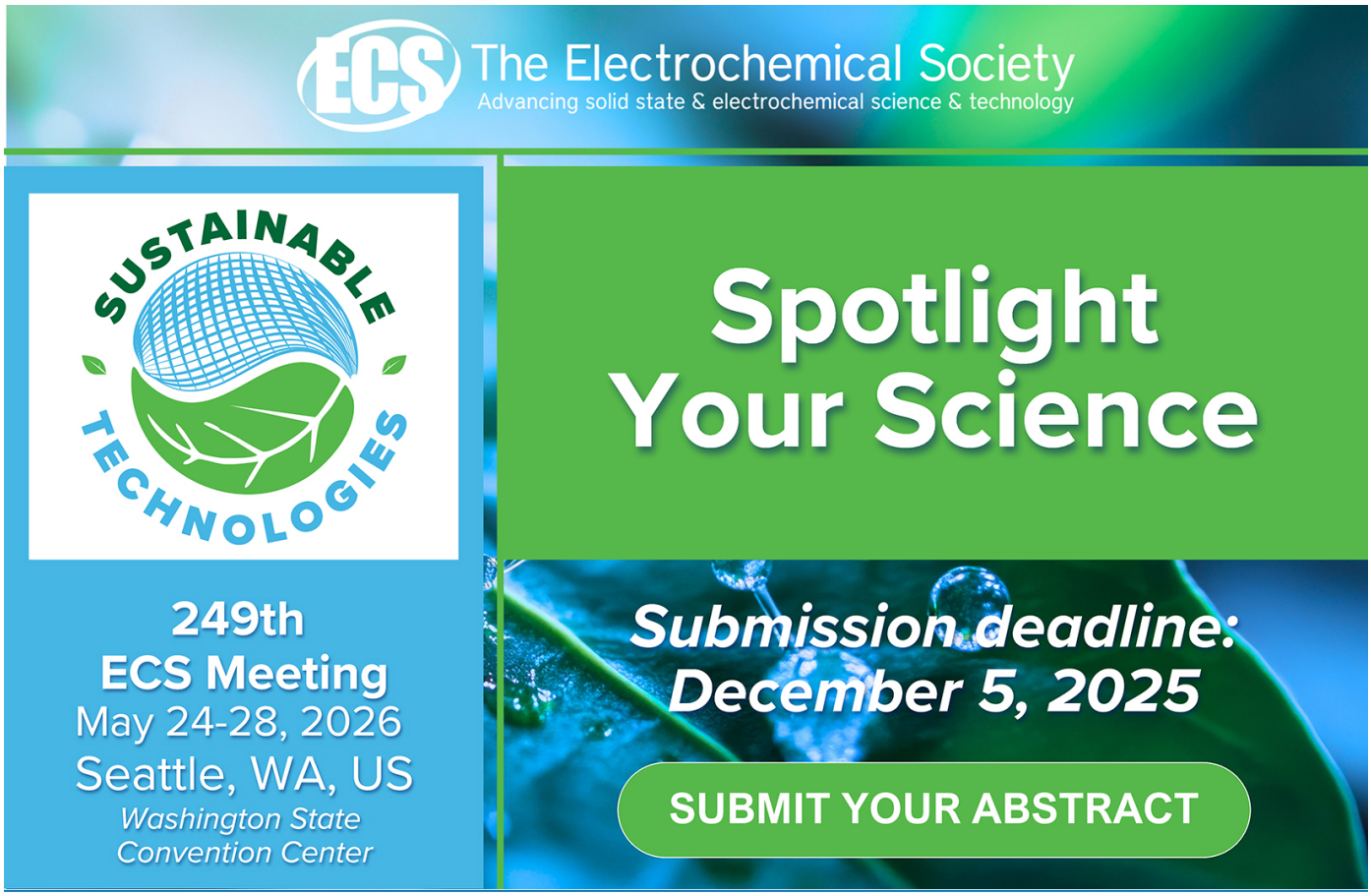

An intense electrospray ionization source for soft X-ray photoionization of gas phase protein ions

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Synopsis For gas-phase experiments on complex biomolecular ions, the target density is a most critical issue. We developed a novel high-current electrospray ionization source, delivering 10 times higher currents than conventional systems.

Complementary to conventional biomolecular spectrocopy in the liquid phase, over the past few years the investigation of large and complex biomolecules in the gas phase has gained momentum. Such studies for instance allow to distinguish intrinsic molecular properties from environment effects, to investigate fundamental processes such as nanosolvation, or to benchmark quantum chemical calculations.

The first requirement for experimental studies is non-destructive transfer of fragile biomolecular species (e.g. proteins, DNA) from the liquid phase into the gas phase. Electrospray ionization (ESI) has proven to be a powerful technique for production of beams of gas-phase biomolecular ions [1]. Despite its versatility, ESI has the major drawback of delivering notoriously low ion fluxes. Typical mass selected biomolecular ion currents obtained with commercial instruments are of the order of few pA - much too low for many applications.

We developed an ESI source, optimized for high ion flux. The source is equipped with a radiofrequency (RF) ion funnel and a housing optimized for efficient pumping. Using a roots pump system then allows the use of a heated capillary with a much larger than usual inner diameter. First tests with the small protein melittin proved, that the source can deliver more than 1 nA of total ions and more than 100 pA of mass selected protein ions.

In a first test, the high flux ESI source was interfaced with the NanoClusterTrap [2] setup at the Helmholtz Zentrum Berlin (HZB). Here, electrosprayed melittin cations were RF guided, mass selected and eventually accumulated in a cryogenic linear RF ion trap. The trapped cations were then exposed to soft X-rays from the HZB UE52_PGM beamline.

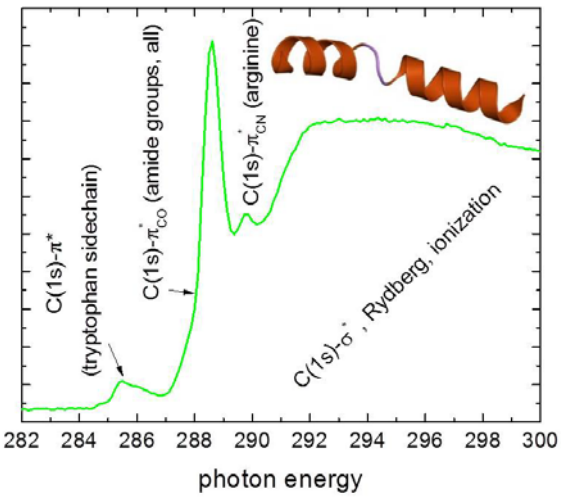

Figure. Fragment yield for $(melittin+2H)^{2+}$ after soft X-ray absorption at the C K-edge.

Preliminary results for photoionization of $(melittin+2H)^{2+}$ are displayed in figure. The quality of the data renders for instance circular dichroism studies feasible.

References

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[2] J. T. Lau, J. Rittmann, V. Zamudio-Bayer, M. Vogel, K. Hirsch, Ph. Klar, F. Lofink,T. Möller, B. v. Issendorff, Phys. Rev. Lett. **101** (2008) 153401

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