

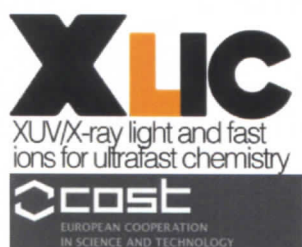
1st Meeting of the XLIC Working Group 2

REACTIVITY OF HIGHLY EXCITED AND HIGHLY CHARGED MOLECULES



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Photoionization of isolated charged proteins – the role of charge state and nanosolvation

A. R. Milosavljević,^{1,*} F. Canon,² V. Z. Cerovski,¹ M. Lj. Ranković,¹
C. Nicolas,³ C. Miron,³ L. Nahon,³ and A. Giuliani^{3,4}

¹*Institute of Physics, University of Belgrade, Pregrevica 118, 11080 Belgrade, Serbia.*

²*INRA, UMR1324 Centre des Sciences du Goût et de l'Alimentation, F-21000 Dijon, France.*

³*Synchrotron SOLEIL, L'Orme des Merisiers, Saint Aubin, 91192 Gif-sur-Yvette, France.*

⁴*UAR 1008 CEPIA, INRA, 44316 Nantes, France.*

*vraz@ipb.ac.rs

Photoionization of isolated protonated peptides and proteins has been studied, particularly the role of either charge state of the precursor or hydration by only a few water molecules. Gas phase VUV and X-ray single-photon photoionization spectroscopy of electrospray-produced protonated bare and nanosolvated biopolymers has been performed by means of coupling a linear quadrupole ion trap with a synchrotron beamline [1].

We have demonstrated, in the VUV photon domain, a strong correlation between the ionization energy of a full protein and both its charge state and structure [2]. This study has been recently extended to inner-shell ionization by soft X-rays. Previously, we have reported the first inner-shell spectroscopy of gaseous protein ions, showing a striking apparent stability of the large photoions arising from direct photoionization or Auger processes [3].

We have also studied the influence of nanosolvation to the physicochemical properties of biomolecules, particularly the susceptibility to VUV irradiation [4]. The measurements have showed that although the nanosolvation of a protonated peptide dimer with only 3 water molecules has a limited impact on the three dimensional structure of this fragile complex, it increases dramatically its stability and prevents apparent photo-fragmentation. The latter experimental results have been confirmed theoretically by using molecular dynamics and density functional theory. This study has been most recently extended to AMP nucleotide and the role of a single solvent molecule.

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References

- [1] A.R. Milosavljević et al. *J. Synchrotron Rad.*, **19** 174 (2012).
- [2] A. Giuliani et al. *Angew. Chem. Int. Ed.*, **51** 9552 (2012).
- [3] A.R. Milosavljević et al. *J. Phys. Chem. Letters*, **3** 1191 (2012).
- [4] A.R. Milosavljević et al. *Angew. Chem. Int. Ed.*, **52** 286 (2013).