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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

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Photoionization of isolated protonated peptides and proteins has been studied, particularly the role of either charge state of the precursor or hydratation by only a few water molecules. Gas phase VUV and X-ray single-photon photoionization spectroscopy ofelectrospray-producedprotonated bare and nanosolvatedbiopolymers 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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