# Influence of nanohydration on the structure and radiation-induced fragmentation of gas-phase biomolecules

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**Abstract**
In the biological medium, water conditions the structure and function of biomolecules, with the first solvation shell playing a fundamental role in these properties. To understand this particular role of water, a bottom-up approach can be utilized, such as investigating the stepwise hydration of biomolecules in the gas phase. This thesis presents an experimental and theoretical study on the influence of nanohydration on the structure and physical processes of gas-phase biomolecules by irradiation with soft X-ray photons. First, we described the experimental setup and the electrospray ionization source dedicated to producing nanohydrated biomolecules. In the second part, we studied the solvation of two model systems: deprotonated adenosine monophosphate (AMP) and protonated phosphorylated amino acid phosphotyrosine. Using quantum chemical calculations, we investigated the influence of stepwise solvation on the three-dimensional structure and spectroscopic characteristics of AMP. We demonstrated that a single water molecule already affects the geometry. Furthermore, we investigated the influence of a single water molecule on the structure and X-ray absorption spectra of phosphotyrosine. By combining soft X-ray spectroscopy with quantum chemical calculations, we could determine the location of the water molecule and demonstrate its features in the X-ray absorption spectrum at the oxygen K-edge. Lastly, we examined the electronic fingerprint of the protonation sites in model peptides using their X-ray spectra at the nitrogen K-edge. We mapped the differences in the electronic transitions caused by different proton locations at the nitrogen and oxygen sites present within the peptide backbone and amino acid side chains.