

# Physikalisches Kolloquium

Thursday, 16.11.2017, 17:15, HS 100

Reception with coffee & cookies 16:45

(For university staff: please bring your own cup for sustainability reasons)

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## *Photoemission spectroscopy from aqueous solutions*

### Abstract

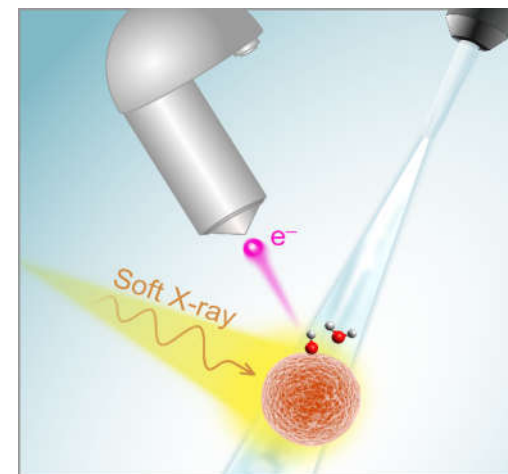
Applications of soft-X-ray resonant and non-resonant core-level photoelectron (PE) spectroscopy to liquid microjets for the study of the electronic structure of aqueous solutions are presented. Several examples are discussed, including atomic transition-metal (TM) ions, TM-oxide nanoparticles (NPs) dissolved in water, and hydrogen-bonding molecules. Exemplified for  $\text{Fe}^{2/3+}(\text{aq})$  we show that the non-radiative (autoionization) relaxation processes following resonant TM 2p excitation uniquely reveal details on the bonding interactions of the metal-aqua complexes. Our interest in the NPs is the electronic structure of the NP – aqueous solution interface, and particularly the detection of dissociated water. Results will be presented for 6-nm  $\text{Fe}_2\text{O}_3$  NPs.

The shape of Auger-electron spectra was observed to be sensitive to the participation of solvent water in the relaxation process. For instance, the high-energy tail of the oxygen 1s Auger electron spectrum from liquid water reveals an electronic de-excitation process of core-level ionized water in which a pairs of cations form, either  $\text{H}_2\text{O}^+\cdots\text{H}_2\text{O}^+$  or  $\text{OH}^+\cdots\text{H}_3\text{O}^+$ .<sup>1</sup> These reactive species are expected to play a considerable role in water radiation chemistry and biodamage. Isotope measurements show that autoionization also occurs from a series of transient Zundel-type structures evolving from proton transfer, from the ionized water molecule to a neighbor molecule, within a few femtoseconds. The actual autoionization is either through intermolecular Coulombic decay (ICD) or Auger decay.<sup>1,2</sup> These so-called proton-transfer mediated charge separation (PTM-CS) processes are found to also occur in other and similarly hydrogen-bonded solute molecules such as  $\text{NH}_3(\text{aq})$ ,  $\text{NH}_4^+(\text{aq})$ , or  $\text{H}_2\text{O}_2(\text{aq})$ .<sup>3</sup>

<sup>1</sup> S. Thürmer et al., *Nat. Chem.* **5**, 590-596 (2013).

<sup>2</sup> P. Slavicek et al., *J. Am. Chem. Soc.* **136**, 18170–18176 (2014).

<sup>3</sup> P. Slavicek et al., *J. Phys. Chem. Lett.* **7**, 234–243 (2016).



All of you interested in physics are cordially invited!

Contact: Dr. André Knie, Experimental Physics IV, More Information: [uni-kassel.de/go/physikalisches\\_kolloquium](http://uni-kassel.de/go/physikalisches_kolloquium)