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Electronic structure and excited state reactions of molecules in aqueous solutions studied by time-resolved XUV photoelectron spectroscopy

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We report on the state-of-the-art time-resolved photoelectron spectroscopy (LJ-TRPES) of molecular chromophores solvated in aqueous environment using wavelength-selected XUV pulses from high-order harmonic generation and micro-liquid jet (LJ) technology. LJ-TRPES is one of the most direct analytic methods to follow transient electronic structures of complex photoexcited molecules.

In one example, we investigate in combination with conventional time-resolved transient absorption spectroscopy (TAS) the relaxation timescales as well as absolute binding energies of the electronic states of Metanil Yellow (MY), an aminoazobenzene derivative. The excited-state dynamics obtained with both methods is compared to time-dependent density functional theory (TDDFT) calculations. As shown in previous work, the low-energy part of the absorption spectrum of MY consists of two overlapping bands, associated with the hydrated and non-hydrated forms of the dye, with maxima at 416 and 464 nm, respectively. Using TAS and TRPES with different excitation wavelengths (λ=370 nm and λ=490 nm), we reveal that both forms undergo similar dynamics characterized by ~1.5 ps time constant reflecting internal conversion to the trans ground state along the torsional coordinate.

In the other example we investigate with TRPES the ultrafast relaxation of NAIP, biomimetic molecular switch. In TAS experiments the switch demonstrates an almost ballistic approach to the conical intersection(CINT) and thus is a good candidate for observing passage of CINT by TRPES.

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