

# Photoinduced Proton Transfer Dynamics in Aqueous Urea Solution Probed by Water-Window X-ray Absorption Spectroscopy

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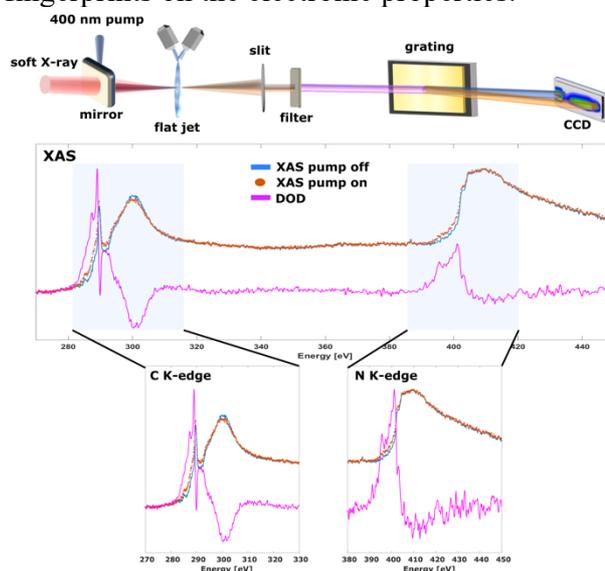
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In this work, we present femtosecond time resolved X-ray absorption spectroscopy (trXAS) of aqueous urea ( $\text{CH}_4\text{N}_2\text{O}$ ) solution utilizing a high-harmonic-generation (HHG) source covering the essential carbon and nitrogen edges as depicted in Figure 1. The inherently broadband HHG pulse allows to probe both edges simultaneously and is therefore ideal for XAS [1]. XAS is an element and site-specific method and very popular in investigating the electronic properties of matter including intermolecular dynamics in a liquid environment [2,3]. Another advantage of the experimental set-up is that the pump and probe pulse are derived from the same source and therefore are intrinsically time-jitter-free. Furthermore, we utilized a sub- $\mu\text{m}$  thin flat jet to record artefact free XAS in transmission mode [4]. Our experimental results indicate spectral features appearing after  $\sim 200$  fs and lasting up to around 700 fs before it stabilizes, which we attribute it to nuclear rearrangement after multiphoton ionization. Theoretical simulation and XAS calculations of several urea dimer and urea-water geometries support the experimental findings and can reproduce the main spectral features. Furthermore, the theoretical results indicate charge dynamics

changing the structural arrangement and leaving geometric specific spectral fingerprints on the electronic properties.



**Figure 1. Top:** A schematic illustration of the experimental scheme. An intense 400 nm pump creates a valence hole on the sample provided by a liquid flat-jet, and then probed by a delayed soft X-ray pulse. **Middle:** The X-ray absorption spectrum of 10 M urea solution at the carbon and nitrogen K-edges with, without pump and the integrated difference (pink). **Bottom:** Zoomed in on the carbon and nitrogen signal.

## References

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