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A study of the dynamical energy flow in uracil

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Synopsis The time resolved photoionization of C 1s in uracil following excitation of the neutral molecule by 260 nm pulses has been studied at LCLS.

Uracil, is one of the building blocks of RNA and is closely related to thymine, one of the letters in the DNA alphabet. A fundamental question in ultrafast photodynamics of these molecular subunits is: how do they resist damage due to the strong absorption of UV radiation? Pyrimidine and purine derivatives, the main components of DNA bases, can dissipate dangerous electronic energy before it causes bond breakage and consequent errors in the DNA code. Current theories focus on conical intersections of the excited state, and the roles of allowed and dark excited states.

We have investigated the dynamics of core ionized uracil by time-resolved pump-probe techniques, using a femtosecond laser system as the pump and the X-ray pulse of the LCLS as probe, combined with an efficient electron detector: a magnetic bottle. By laser pumping the ground state of the molecule and probing the excited states with core level spectroscopy, one can shed light on the nature of internal electronic energy conversion after UV photoexcitation. In the experiments the photoionization of C1s at 350 eV has been studied at different delay times between the UV excitation (260 nm, ππ* excitation) and the X-Fel ionisation pulses. The operating conditions of LCLS have been chosen in order to avoid non-linear processes. The difference between the spectra with laser on and off is shown in figure (1b). In the figure a fast sub 100 fs dynamics and a slower one can be easily identified.

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Figure 1. (a) Calculated XPS spectra of the ground and two excited states of uracil. (b) Difference between the measured photoelectron spectra with and without ultraviolet excitation as a function of the delay