

Ultrafast bond deformations in molecular systems investigated with soft X-ray spectroscopy

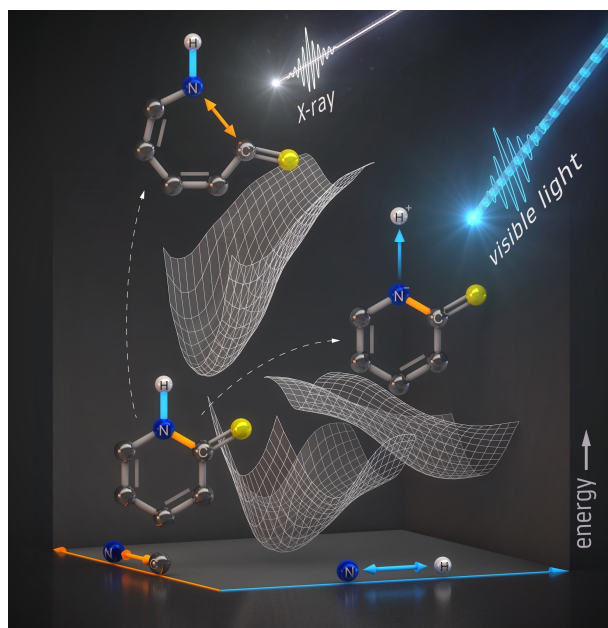
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Ultrafast excited state proton transfer (ESPT) processes are discussed as photo-protection mechanisms in bio-molecules e.g. DNA [1] and melanin [2]. We demonstrate the applicability of N 1s X-ray absorption spectroscopy (XAS) and resonant inelastic X-ray scattering (RIXS) to investigations of ESPT processes by establishing spectral fingerprints for N protonation in the cyclorganic ESPT compound 2-Thiopyridone. [3,4] Its ultrafast response to photo-excitation is investigated in the first time-resolved N 1s RIXS measurement of a dilute molecular system in solution performed at the LCLS. [4] Spectroscopic signatures indicating N deprotonation are identified within the first 100 femtoseconds after the optical excitation. N 1s core excitation is found to induce dynamics along the N-C bond. In complementary investigations at the synchrotron BESSY II, pico- to nanosecond dynamics are accessed in a dedicated photochemistry end-station for transient transmission XAS [5].



Ultrafast photon energy dependent bond deformation in 2-Thiopyridone. Optical excitation induces N-H dynamics on femtosecond timescales, whereas the system is promoted to a N-C dissociative potential upon N 1s core-excitation.

References

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