Abstract Submitted
for the DAMOP19 Meeting of
The American Physical Society

Thionated Uracils under UV Irradiation: Intramolecular Effects on the Intersystem Crossing Dynamics[1] SUSANNE ULLRICH, Univerisity of Georgia, Department of Physics and Astronomy, ABED MOHAMMADZADE, Univeristy of Georgia, Department of Physics and Astronomy — The canonical nucleobases, which form the building blocks of our genetic coding material, are known to protect themselves against photodamage through ultrafast internal conversion processes that dissipate potentially harmful UV energy into heat. However, seemingly minor changes such as single atom substitutions can profoundly alter the photophysics of the nucleobases. In thiobases, where an oxygen is replaced by sulfur, these internal conversion pathways are inaccessible and crossing onto the triplet manifold becomes highly efficient. While long-lived, reactive triplet states, as observed in some of the thiobases, negate their photoprotection, these properties are highly desirable for pharmacological applications, e.g. as photosensitizers in cancer treatments. Using time-resolved photoelectron spectroscopy the response of a series of thiouracils to UV irradiation has been investigated to unravel the mechanistic details governing their unique ultrafast intersystem crossing dynamics. Remarkable differences are observed for 2-thiouracil, 4-thiouracil and 2,4-dithiouracil when the degree of thionation and position of sulfur atom is altered.

[1]NSF CHE-1362237 and CHE-1800050

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Date submitted: 01 Feb 2019 Electronic form version 1.4