



Contribution ID: 155

Type: Contributed poster

Ultrafast Auger spectroscopy of UV excited thymine

Monday, 25 June 2018 18:45 (15 minutes)

Excited molecules can reconvert their excitation energy into other types such as electronic, chemical or thermal energy. The relevant molecular processes are ultrafast and often involve coupled electronic and nuclear dynamics not fulfilling the Born-Oppenheimer approximation. Their experimental investigation is complicated by the existence of dark S_1^* states if the molecule contains heteroatoms. One such chromophore is the model system thymine.

It has been studied with a variety of time-resolved methods including non-resonant Auger and NEXAFS spectroscopy [1,2]. From the former study, it was concluded that the relaxation of UV-excited thymine involves a $S_1^* \rightarrow S_0$ transition through a conical intersection. The internal conversion into this S_0 state was observed in integrated Auger spectra of the latter study and determined to happen on a timescale of (60 ± 30) fs. The S_0 feature then further decays biexponentially with time constants of (1.9 ± 0.1) ps and (10.5 ± 0.2) ps.

We show energy resolved Auger spectra of thymine at resonant absorption lines in NEXAFS spectra after excitation with ultraviolet light and discuss their sensitivity on the molecular relaxation process.

Full author list: see [2] and Jan Metje.

[1] McFarland et.al., Nature Comm. 5:4235, 2014

[2] Wolf et.al, Nature Comm. 8:29, 2017

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Session Classification: Poster session