

Simulating Ultrafast Photoexcitation Dynamics in Gas- and Liquid-Phase Furfural

Ultrafast ring-opening dynamics is considered an important channel for the non-radiative decay of an electronically excited state in a number of molecules.

In this project, the ultrafast ring-opening of furfural triggered by a 266nm UV-light pulse is studied theoretically. It is explored how the photo-induced dynamics can be probed using ultrafast XUV absorption spectroscopy.

The project involves a modelling of the dynamics and the probe step in the gas phase as well as the liquid phase. It will allow to interpret available experimental results.

Group

FS-CFEL-3

Project Category

A6. Theory and computing

Special Qualifications

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