CFEL
SCIENCE

SEMINAR

21 April 2022, 10:00–11:00h
CFEL - Building 99, seminar room I and II (ground floor)
online: https://desy.zoom.us/j/99570520017 (password: 911851)

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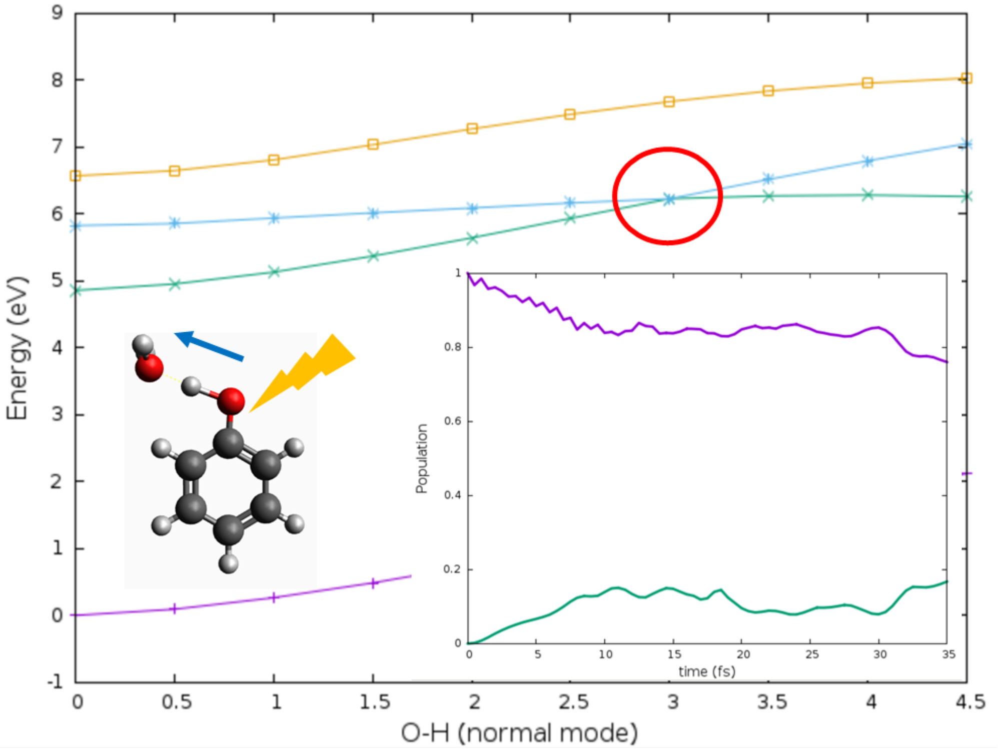
Why does the photochemical reaction of phenol become ultrafast at the air–water interface?

Recent work by Kusaka *et al.* [1] using femtosecond time-resolved vibrational spectroscopy has shown that the photochemical hydrogen dissociation of phenol at the air-water interface proceeds 10^4 times faster than in the bulk aqueous phase. It was suggested that the interface provides a distinct reaction environment which modifies the electronic states of phenol allowing for faster H dissociation via the $\pi\pi^*$-$\pi\sigma^*$ conical intersection.

We have investigated this process theoretically using time-dependent quantum dynamics simulations. Building on previous work for gas phase phenol [2], the on-the-fly Direct Dynamics variational Multi-Configurational Gaussian (DD-vMCG) method has been applied to phenol-H_2O and phenol-$(H_2O)_2$ clusters on excited electronic states. The results of these simulations will be discussed in the context of the spectroscopy experiments. It will be shown that they suggest a different explanation for ultrafast phenol dissociation at the air-water interface than was suggested by Kusaka *et al*.

1. Kusaka, R., Nihonyanagi, S. & Tahara, T., *Nat. Chem.* **13,** 306–311 (2021)
2. Christopoulou, G., Tran, T. & Worth, G. A., *Phys. Chem. Chem. Phys.* **23**, 23684-23695 (2021)

Host: Jochen Küpper/ CFEL Molecular and Ultrafast Science Seminar


Energy (eV)
9
8
7
6
5
4
3
2
1
0
-1
0
0.5
1
1.5
2
2.5
3
3.5
4
4.5
O-H (normal mode)
Population
1
0.8
0.6
0.4
0.2
0
0
5
10
15
20
25
30
35
time (fs)