

**21<sup>st</sup> June 2023 - 2:00 p.m.**  
CFEL-bldg. 99, seminar room IV

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## The race between proton and electron transfer: theory view

In this talk, I will present our ongoing efforts to model coupled electron-nuclear dynamics in highly excited molecules and materials. While the primary emphasis will be on proton transfer dynamics, I will also address electron transfer and electron-induced reactivity. I will begin by examining the proton transfer of water upon upper valence ionization, recognized as the fastest acid-based reaction. Utilizing X-ray free electron laser technology, we are able to directly track the proton transfer process. I will highlight the role of non-adiabatic and nuclear quantum effects in this reaction, along with the relationship between these findings and recent strong-field experiments. Next, we will delve into the interplay between proton and electron processes in various phenomena: radiolytic formation of solvated electron, non-local Auger processes such as intermolecular Coulombic decay (ICD) or multiply ionized systems. I will end up with analogical processes for chemically more interesting systems (Figure 1). The talk will conclude with broader considerations. Firstly, numerous novel phenomena have

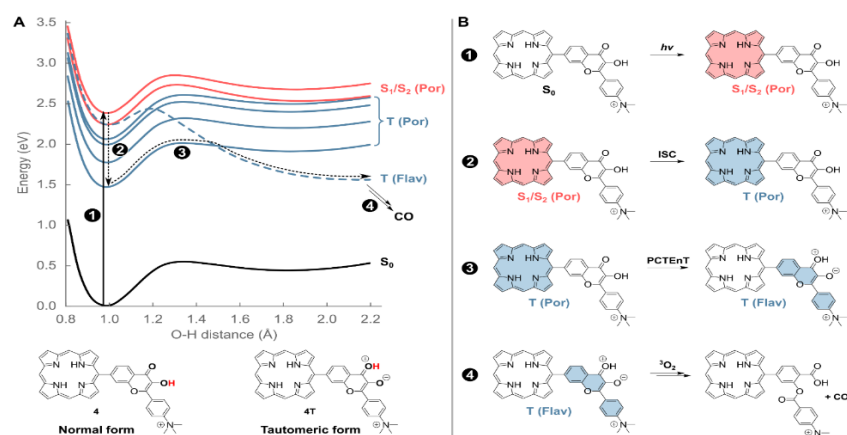


Figure 1. Proton coupled energy transfer

recently emerged in the field of X-ray molecular science. However, this knowledge has yet to permeate other research areas, such as radiation chemistry, biophysics, and astrochemistry. Secondly, I will discuss the available toolbox for modeling complex photon and electron-induced processes in condensed phases.