# SIMULATING VIBRATIONAL ENERGY TRANSFER THAT PROMOTES EXCITED STATE PROTON TRANSFER IN PYRANINE

JUSTIN J TALBOT, JAMES SHEE, MARTIN HEAD-GORDON, *Chemistry, University of California, Berkeley, Berkeley, CA, USA*; CLAUDIUS HOBERG, MARTINA HAVENITH, *Physikalische Chemie II, Ruhr University Bochum, Bochum, Germany*.

Identifying molecular-level details of the solvent reorganizations that facilitate photo-induced excited-state proton transfer is challenging for current experimental and theoretical approaches. One distinct challenge for computations is accessing the long time scales required to get frequency-resolved data. In this talk, I will discuss our recent work modelling optical pump THz probe experiments using molecular dynamics simulations to elucidate the ultrafast changes in the solvation environment for three derivatives of pyranine: the photoacid HPTS, the methoxy derivative MPTS, and the photobase OPTS. The experiments show damped oscillations in the THz signal at short times for all three derivatives and our simulations enable their assignment to vibrational energy transfer beatings between the photoexcited chromophore and nearby solvent molecules. Additionally, the simulations of HPTS reveal strikingly efficient sub-ps energy transfer into a particular solvent mode, that is active near 4 THz, and which can provide the requisite energy required for solvent reorganization promoting proton transfer.