ULTRAFAST SPECTROSCOPIC AND AB INITIO COMPUTATIONAL INVESTIGATIONS ON SOLVATION DYNAMICS OF NEUTRAL AND DEPROTONATED TYROSINE.

TAKASHIGE FUJIWARA, Center for Photochemical Sciences, Bowling Green State University, Bowling Green, OH, USA; MAREK Z. ZGIERSKI, Steacie Laboratory, National Research Council of Canada, Ottawa, ON, Canada.

We have studied one of the aromatic amino acids, tyrosine, regarding its photophysical properties in various solvent conditions by using a femtosecond fluorescence up-conversion technique and high-level TDDFT and CC2 computations. In this talk, profound details not only on ultrafast solvation dynamics on a neutral tyrosine in various solvents, but also on the excited-state dynamics for a single- (or doubly-) deprotonated tyrosine under various pH solutions will be presented. In high basicity, a tyrosine shows different absorption/emission spectra, and a total spectrum consists of a combination of these individual spectra that depend on the pH of the solution. The time scale of acid–base equilibrium is essential in solvation dynamics; whereas the protonation is simply controlled by diffusion, the de-protonation is considered to be slow process such that acid–base equilibrium may not be reached in the short-lived excited state after photo-excitation. Experimental and computational approaches taken and insights obtained in this concerted work will be described.