SIMULATING THE ELECTRONIC SPECTRA OF AROMATIC CHROMOPHORES IN AQUEOUS SOLUTION

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I will discuss our recent efforts to understand the absorption and fluorescence spectra of small aromatic chromophores (such as uracil and phenol) in aqueous solution. Our approach is to utilize quantum chemistry to predict the excited states of the chromophore embedded in a reasonably large water cluster (> 70 H_2O molecules, in some cases). In uracil, there is an important question regarding whether solvent can alter the energetic ordering of the close-lying bright ($^1\pi\pi^*$) and dark ($^1n\pi^*$) states. More generally, we are interested in the extent to which "micro-hydration" studies (which include only those water molecules that are directly hydrogen-bonded to the chromophore) are sufficient to predict the spectroscopy in bulk water.