UNDERSTANDING SOLVENT EFFECT ON THE FLUORESCENCE SPECTRA OF 4-VINYL-N,N-DI(P-TOYLY)ANILINE DERIVATIVES

THOMAS T TESTOFF, *Department of Chemistry and Biochemistry, Southern Illinois University, Carbondale, IL, United States*; LICHANG WANG, *Department of Chemistry and Biochemistry, Southern Illinois University Carbondale, Carbondale, IL, USA*.

DFT calculations were carried out to obtain the absorption and fluorescence spectra of 4-vinyl-N,N-di(p-toyly)aniline derivatives denoted as MTPAs, in different solvents to understand the correlation between the functional groups and solvent effects. In this presentation, we will discuss DFT results on six MTPAs in two solvents, dichloromethane and toluene, and the solvent impact on the structures of electronically excited states. We will also briefly discuss the choice of functional of the DFT results with comparison to the experimental measurements of these derivatives.