# DFT and TDDFT study some pyrene derivatives in excited state

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This study presents a computational investigation of Pyrene and its -OH, $-NH_2$, and -CN, substituted derivatives at position 1 in gas phase and in different solvents in excited S_1 state. Calculations were performed by density functional theory (DFT) with the B3LYP functional, where 6-311++G(d,p) basis set employed for 1-substituted Pyrene derivatives. Time-dependent density functional theory (TDDFT) with the same functional and basis set was used for the analysis of excited states of molecules and emission spectra. 40 lowest singlet excited states were calculated for each molecule. Molecular orbital energies and the UV-Vis spectra of the studied molecules were illustrated with the same method using the Gaussview program [1] with ground state geometries. The total electron density surfaces of pyrene and its derivatives mapped with the electrostatic potential values in gas state and various solvents for the excited state equilibrium geometry were shown below. Similar to the observation in our former study [2], there is a charge transfer from the pyrene ring to the electron withdrawing CN group (red: negative electron density). The Polarizable Continuum Method (PCM) [3, 4] have been applied for all gas phase optimized structures to evaluate the solvation effect on the transitions of the investigated molecules in nonpolar (CH, cyclohexane), medium polar (THF, tetrahydrofuran) and polar solvents (ACN, acetonitrile and H_2O, water).
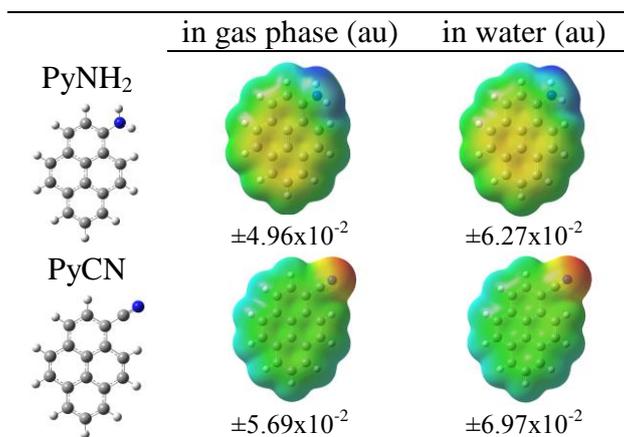
The results showed that the stability of the investigated systems increased with increasing solvent polarity. E_{00} energies and fluorescence lifetimes were calculated using computed emission spectra. All calculations were performed using Gaussian09 software [5].

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