STUDY OF AGGREGATION OF THE 2,7'-DICHLOROFLUORESCEIN DYE CAUSED BY THE INTERMOLECULAR HYDROGEN BOND

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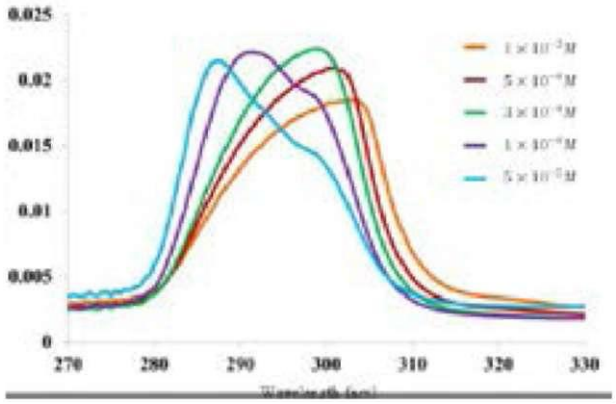
Introduction. The project's main objective is to study the aggregation of the 2',7'-dichlorofluorescein dye molecule through intermolecular hydrogen bonding in various solvents. With two chromophores perpendicular to each other, 2',7'-dichlorofluorescein likely demonstrate J-aggregate and H-aggregate simultaneously. The present project is expected to provide some insights in the knowledge-based molecular design to improve device performance for optoelectronic applications.

Materials and methods. 2',7'-dichlorofluorescein solvents were purchased from the Sigma Aldrich without further purification. Cary 100 UV-Visible spectrometer and the Hitachi F-700 fluorescence Spectrometer were used to obtain the UV-Vis absorption and fluorescence spectra. Three solvation models were applied to the monomer and dimer models ofthe dye, namely: implicit, explicit, and hybrid (implicit-explicit) solvation models. All ground-state geometries were done using density functional theory (DFT) without any symmetry constraints and the excited state energies were calculated using time-dependent DFT.



Results and discussion. The UV-Visible spectra in various solvent generally show two absorption bands corresponding to two chromophores. The fluorescence of 2',7'-dichlorofluorescein in methanol, ethanol, and acetonitrile was quenched at the higher concentration. The fluorescence quenching as well as the multi components in the UV-Visible absorption were contributed to the dye molecule aggregation through intermolecular hydrogen bond especially in methanol, ethanol, and acetonitrile. As water can form stronger hydrogen bond with the dye molecule, the highly hydration in the aqueous phase stopped the dye molecules from aggregating. DFT calculation convinces the intermolecular hydrogen bond among the dye molecules. The simulated UV-Visible transitions are consistent with the experimental results.

Conclusions. Both experimental (UV-Vis and fluorescence) results and DFT calculation indicate that the molecules of 2',7'-dichlorofluorescein can form intermolecular hydrogen bond. The hydrogen bonding based aggregated dye molecules exhibit special dilution features on the corresponding UV-visible and fluorescence spectra. The theoretical calculation supports the proposed aggregation mode.

References.

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