Theoretical analysis of environmental effects on excited-state properties

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The excited-state properties of molecules are affected by their environment such as solvent and counter ion. However, it is often difficult to explain the molecular mechanism. We have been studying such environmental effects on the excited-state properties by using quantum chemical calculations and appropriate solvent models. In this presentation, we will talk about our recent progresses. For example, we investigated the solvent dependency of excited-state intramolecular proton transfer (ESIPT) in 2-(2′-hydroxyphenyl)-benzothiazole. It was found that the hydrogen-bond acceptability of solvent plays important roles in ESIPT. We also investigated the solvent and anion dependency of fluorescence quenching of a phospholium cation. The charge-transfer state of the cation-anion complex was found to be responsible for the dependency. In addition, we will talk about the solvent dependency of the fluorescence spectrum of pyrene-MoS_2 nanosheet system.