Vibronic Coupling Density and Its Applications

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Vibronic couplings play important roles in various properties of molecules. In a light-emitting molecule, for instance, off-diagonal vibronic couplings give rise to nonradiative transitions, and a diagonal vibronic coupling is a driving force of the vibrational relaxation from a vertical excited state. A large vibrational relaxation results in small Franck-Condon factors which give rise to a small rate constant of the radiative transition. Therefore, small diagonal and off-diagonal vibronic couplings are crucial in designing of an efficient emitting molecule[1].

We have proposed a concept of vibronic coupling density (VCD) to analyze and control diagonal and off-diagonal vibronic couplings[2,3]. On the basis of VCD analysis, we designed efficient emitting molecules by the suppression of vibronic couplings in anthracene[4] and triphenylamine[5], and we observed the increase of quantum yields of the designed molecules[6,7]. It should be noted that triphenylamine is a non-emitting molecule. We can make a non-emitting molecule fluorescent by the molecular design on the basis of VCD analysis.

Thermally-activated delayed fluorescence (TADF) has attracted much attention as a highly-efficient emitting mechanism for organic light-emitting diodes[8]. In this mechanism, both T_1 and S_1 excitons which are generated by electrical excitations are utilized for light emission. Thermally excited T_1 excitons are converted to S_1 excitons via reverse intersystem crossing (RISC). We will discuss that highly-efficient light-emission via RISC from T_n states higher than T_1 is possible by suppressing non-radiative transitions from T_n based on the concept of vibronic coupling density[9,10].

We will also discuss a design principle of carrier-transporting molecules using the VCD concept, and VCD as a chemical reactivity index.

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