Manipulation of peripheral donor and acceptor substituents in emitter-layer materials toward highly efficient and stable OLEDs

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論 文 名　：Manipulation of peripheral donor and acceptor substituents in emitter-layer materials toward highly efficient and stable OLEDs
（高効率及び高耐久 OLED を目指した発光層材料のドナー・アクセプター置換基の操作）

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論　文　内　容　の　要　旨

This thesis presented thermally activated delayed fluorescence (TADF) emitter and host materials to boost the efficiency and stability of TADF OLEDs. Because of their high stability and efficiency, D-A-type compounds are one of the most promising TADF material families. We explored the relationship between molecular architectures and photophysical parameters including k_{RISC} and device durability. By comparing the stabilities of different TADF molecules, we unlocked the potential for generating new TADF materials. Additionally, the outcoupling efficiency lowers the EQE to 20–30% even if the IQE of OLEDs may approach 100% using singlets and triplets in TADF OLEDs. The host molecule is essential for improving the guest molecule's molecular orientation in the EML. We introduced a host material with great thermal stability and triplet energy, which leads to better orientation of diverse guest materials.

In Chapter 1, I described the general introduction to organic light-emitting diodes (OLEDs), how molecular structure affects the properties in TADF OLEDs, and how the horizontal orientation enhances the outcoupling efficiency in OLEDs. Then, I discussed the molecular orientation approximations at the beginning of OLED research and recent research. Lastly, I described the aim and outline of the thesis.

In Chapter 2, I designed a new TADF material with multiple D-A type structures and a hetero-donor design that uses two different donor units, DMAC and Cz. The newly designed emitter showed high PLQY under different circumstances, including polar media and high doping concentrations. The EQE of OLEDs was rather high in p-type hosts mCBP, CCP, and n-type host PPT. Furthermore, I determined that multiple D-A-type molecules have higher photostability than single D-A-type molecules. However, additional critical factors might have an impact on OLED operating stability.

In Chapter 3, I presented a new molecule, 6CzPh, as a host. Compared to typical host

materials, 6CzPh, an undiscovered carbazole derivative in OLEDs, has exceptional qualities as a host. According to our research, 6CzPh is a viable option for OLED applications. The new host's high triplet energy and robust structure help to achieve high EQE and device stability. The host material enhanced the horizontal molecular orientation of several guest emitter types and their intrinsic properties. Notably, the disk-shaped 4CzIPN emitter showed a fully horizontal molecular orientation with the new host 6CzPh.

In Chapter 4, I concluded the thesis and described the main findings of each chapter. Then I described the future perspectives of my studies. In organic lasers, our prime goal is to realize more stable OLEDs with high efficiencies. This study features symmetric molecules with bulky donor units connected through a phenyl ring. Generally, all muli-donor/hetero-donor TADF molecules are based on carbazole-based donor units. I introduced acridine (DMAC) as a donor in a hetero-donor-designed emitter. DMAC is a donor that has a strong donor strength; it has a crowded structure that provides the steric effect, and the highly twisted DMAC could offer a small ΔE_{ST}. Furthermore, although the IQE of OLEDs can reach 100% by utilizing singlets and triplets in TADF OLEDs, the outcoupling efficiency reduces the EQE to 20-30%. It is well known that the host molecule plays a key role in achieving better molecular orientation of the guest molecule in the emissive layer (EML). Here, I present a host material with high thermal stability and triplet energy, which results in improved orientation of various guest materials. Finally, I proposed methods to enhance the stability and performance of 2Cz2DMAC2BN emitter-based OLEDs and uses of the host 6CzPh in different OLED systems.