Studies on Photophysical and Electrical Characteristics of Host-Guest Systems in Organic and Organic-Inorganic Hybrid Thin-Films

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論 文 名　：Studies on Photophysical and Electrical Characteristics of Host-Guest Systems in Organic and Organic-Inorganic Hybrid Thin-Films
（有機及び有機-無機ハイブリッド薄膜におけるゲスト-ホストシステムの光物性及び電気物性に関する研究）

区　　分　：甲

論 文 内 容 の 要 旨

Thesis summary :

Luminescent materials, which emit light when stimulated by an external energy source, have revolutionized various fields of science and technology. Their ability to convert energy into visible light has made them indispensable in applications such as lighting, displays, sensors, and optoelectronic devices. One approach to enhance the luminescent properties and functionality of these materials is through the utilization of Host-Guest (H-G) systems. H-G systems have many advantages for luminescent materials, primarily by providing a favorable environment for luminescent guests, thereby enhancing their luminescence efficiency.

In **chapter 1**: I briefly introduced the general introduction of the luminescent materials and explained the advantages of H-G system from organic to organic-inorganic hybrid system. On the one hand, organic materials, including, small organic molecules, and organic dyes, have shown great potential for devices like OLEDs, OSCs, and biological imaging tools. On the other hand, the integration of organic luminophores into inorganic host materials has led to the emergence of organic-inorganic hybrid H-G systems. These systems combine the desirable properties of both organic and inorganic components, offering enhanced luminescent properties and functionality. Despite significant progress, the development of high-efficiency luminescent materials remains a crucial focus. Inspired by this motivation, this dissertation is dedicated to designing luminescent materials in H-G systems from organic-organic to inorganic-organic approaches, and investigating their application for light emission. The goal is to demonstrate the unique advantages of organic-organic and organic-inorganic hybrid H-G systems for light emission.

in **Chapter 2**: we introduced a deuterated host, PYD2Cz-d16, and a TADF green emitter, 4CzIPN, to form an organic-organic H-G system. We found that the photophysical properties of the H-G system based on deuterated PYD2Cz-d16 are similar to that of the non-deuterated PYD2Cz host. More importantly, deuterated PYD2Cz-d16 forms a denser film than PYD2Cz, resulting in different carrier transport properties as demonstrated by HODs/EODs. The green device using the deuterated H-G system exhibited enhanced stability (LT95) of 1.7 times longer than that of the PYD2Cz system. The well-balanced carrier transport properties of PYD2Cz-d16 can provide a broad recombination zone, thus increasing the LT95 in OLEDs.

In **chapter 3**: I introduced a novel organic molecule called M1 and its use in fabricating an organic-inorganic H-G structure, M1PB. The chapter examined the thin-film structure, morphology, and crystal structure of this hybrid architecture, as well as its electronic and photophysical properties, through both experimental and theoretical investigations. The charge transport properties of this type II 2D hybrid heterostructure were also probed using HODs/EODs. The results demonstrated that this hybrid material, composed of intertwined M1 and PbBr4 inorganic monolayers, presents two intercalated separate pathways for electrons and holes that can migrate within the inorganic and organic sublayers, respectively. This work provides insight into the band alignment effect on the performance of inorganic-organic H-G systems, which is of paramount importance for future optoelectronic applications.

Chapter 4 extended the previous section. Two major issues need to be addressed for light-emitting applications: exciton dissociation at the Type II heterointerface and limited charge transport in horizontally oriented films. To overcome these challenges, we designed and synthesized new organic fluorophores (BT and 4mBT) with a diamine group and incorporated them into the inorganic framework to form an H-G system. The resulting perovskite films exhibited a type I heterostructure, confining excitons for efficient light-emission, and vertically oriented structures that allow for charge carriers to travel through the inorganic layers between two electrodes. The 2D perovskite films with a type I heterostructure exhibited efficient FRET from the inorganic layer to the organic layer, resulting in high PLQYs. These vertically oriented hybrid H-G systems with efficient interlayer energy transfer hold great potential for optoelectronic device applications.

Chapter 5: In the previous chapter, we successfully fabricated vertically oriented perovskite films containing an inorganic-organic H-G system. However, we found that the PLQY of these perovskite films was lower than that of the pure organic solution. To address this issue, we introduced several host materials into the perovskite structure to form a multi-component H-G system. This approach allowed for the dispersion of the emitter, such as the BT molecule, by the host material, which reduced concentration quenching. Additionally, we investigated the molecular length and energy level requirements of the organic host in the perovskite structure. By carefully selecting the host materials, the multi-component H-G systems showed higher PLQY than the single H-G system, which contains only the inorganic layer and pure emitter layer. This work provides a deep understanding of the critical role played by host materials in organic-inorganic hybrid structures for achieving high PLQY, which is essential for optoelectronic device applications.

In **Chapter 6**: I summarized the design routes to realize high-performance H-G systems for light-emitting applications. Then outlined future challenges that need to be tackled to implement these systems light-emitting applications.