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Development of Pyrimidine-Based Thermally Activated Delayed Fluorescence Emitters Realizing Deep-Blue to Green Emission

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Recently, thermally activated delayed fluorescence (TADF) emitters composed of pure organic compounds have attracted considerable attention because they can realize 100% conversion from electrons to photons without the use of expensive platinum group metals [1]. Indeed, several green emitters have achieved an external quantum efficiency (EQE) of over 30 % in organic light-emitting devices (OLEDs). However, only a few efficient deep-blue TADF emitters have been reported to date. The development of efficient deep-blue emitters is one of the key issues in OLEDs. Here, we developed a series of pyrimidine-based deep blue-to green TADF emitters and manipulating the electronic exited energies. First, we have developed a novel series of TADF emitters called Ac–RPM derivatives using a combination of pyrimidine and acridine [2]. Among them, the optimized Ac–MPM-based OLED showed a light-blue emission realizing a high power efficiency (PE) of 62 lm/W and a high EQE of 25% at CIE of (0.19, 0.37). In addition, we investigated the strucutre–property relationship to unlock the potential of pyrimidine-based emitter [3]. Consequently, we developed a green emitter named PXZ–PPM realizing a PE of over 110 lm/W while maintaining extremely low voltages of 2.2 V at 1 cd/m2 and 3.0 V at 1000 cd/m2 at CIE of (0.36, 0.58). Furthermore, we developed novel pyrimidine emitters called Ac-XMHPMs (X = 1, 2, and 3) containing different numbers of bulky methyl substituents at acceptor moieties, increasing the excited singlet and triplet state energies [4]. Among them, Ac-3MHPM, with a high triplet state energy of 2.95 eV exhibits a high peak EQE of 18% and an EQE of 10% at 100 cd/m2 with CIE of (0.16, 0.15). These efficiencies are among the highest values to date for deep-blue TADF-OLEDs. We believe our molecular design strategy provides fundamental guidance to design novel deep-blue TADF emitters.

References: [1] H. Uoyama, K. Goushi, K. Shizu, H. Nomura, C. Adachi, *Nature* **492**, 234–238 (2012). [2] R. Komatsu, H. Sasabe, Y. Seino, K. Nakao, J. Kido, *J. Mater. Chem.* C. **4**, 2274–2278 (2016). [3] R. Komatsu, H. Sasabe, K. Nakao, Y. Hayasaka, T. Ohsawa, J. Kido, *Adv. Opt. Mater.* **5**, 1600675 (2017). [4] R. Komatsu, T. Ohsawa, H. Sasabe, K. Nakao, Y. Hayasaka, J. Kido, *Appl. Mater. Interfaces* **9**, 4742–4749 (2017).

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