Šiluma aktyvuojamos uždelstosios fluorescencijos valdymas trifeniltriazino-karbazolo junginiuose

Tuning of TADF properties of triphenyltriazine-carbazole derivatives

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Organic light emitting diodes, OLEDs, are undergoing a breakthrough due to a recent discovery of a novel emission mechanism employing delayed fluorescence generated by thermal activation (TADF) allowing to reach 100% internal efficiency without implementing heavy metal atoms in emitter molecules [1], [2].

In the present study, the ability to control the delayed fluorescence properties of donor-acceptor triazinetriphenyl-carbazole derivatives as a function of varying para (**TpCZ**) or meta (**TmCZ**) position of carbazole substituents was investigated. DFT calculations revealed twisted molecular conformations (see Figure 1) for both compounds resulting in a substantial charge transfer (CT) character, and thus in a small singlet-triplet energy gap (ΔE_{S-T}) – a key requirement for efficient TADF process. Investigation of singlet and triplet spectra revealed ΔE_{S-T} of 0.21 eV and 0.13 eV for **TpCZ** and **TmCZ**, respectively.

Highly sensitive photoluminescence measurements allowed an in-depth study of the delayed fluorescence and its temperature dependence. Figure 1 shows luminescence transients of both derivatives. Although, **TpCZ** shows higher fluorescence efficiency, the contribution of delayed fluorescence is much smaller as compared to that of **TmCZ** emission, which mostly originates from TADF. Furthermore, temperature dependent measurements allowed to estimate activation energies E_A for the TADF process, which were found to be 0.20 eV and 0.07 eV for **TpCZ** and **TmCZ**, respectively.



Figure 1. Intensity decay transients of TADF emitters **TpCZ** (filled) and **TmCZ** (empty) as well as chemical structures of both compounds.

Since **TmCZ** showed much more prominent delayed fluorescence, it was chosen as an emitter for the fabrication of TADF OLED. The device structure was as follows: [ITO/m-MTDATA (10 nm)/NPB (15 nm)/mCP (10 nm)/5wt%-**TmCZ**:DPEPO (20 nm)/TPBi (45 nm)/LiF (0.8 nm)/Al (100 nm)], where m-MTDATA, NPB, mCP were used as hole injection and transport, hole transport, hole transport and exciton blocking layers, respectively. TPBi and LiF were used as electron transport and injection layers, respectively.

The device displayed electroluminescence (EL) spectra similar to the corresponding photoluminescence (PL) spectra of **TmCZ**, confirming that EL emission was generated from **TmCZ** via the same radiative decay process as in PL. The EL emission spectrum peak was found to be at 475 nm and the CIE color coordinates were calculated to be (0.16, 0.23), corresponding to a sky-blue emission color. The turn-on voltage of the OLED was found to be in the range of 5-6 V. The maximal obtained EQE for the device was 9.5%. The EQE and luminous efficacy versus current density as well as PL and EL spectra are shown in Figure 2.



Figure 2. EQE and luminous efficacy as a function of current density of the **TmCZ** OLED and the PL and EL spectra of **TmCZ**:DPEPO (dashed) and **TmCZ** OLED (solid), respectively (inset).

Keywords: OLED, thermally activated delayed fluorescence

References

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