Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Supporting Information

Reduction of singlet-triplet energy gap of thermally activated delayed fluorescence emitter by molecular interaction between host and emitter

L. Xie,[a,d] G. Han,[b,c] Y. Chen,[a,c] H. Wang,[a,e] X. Kong,[a,c] X. Wei,[a,c] J. Liu,[a,c] Y. Yi,[b,c] B. Chen,[d] P. Wang,[a,c] and Y. Wang*[a,c]

[a]Key Laboratory of Photochemical Conversion and Optoelectronic Materials, Technical Institute of Physics and Chemistry, Chinese Academy of Sciences, Beijing, 100190, China

[b]Key Laboratory of Organic Solids, Institute of Chemistry, Chinese Academy of Sciences, Beijing, 100190, China

[c]University of Chinese Academy of Sciences, Beijing, 100029, China

[d]College of Life Science and Technology, Beijing University of Chemical Technology, Beijing, 100029, China

[e]Key Laboratory of Synthetic and Natural Functional Molecule Chemistry of the Ministry of Education, College of Chemistry & Materials Science, Northwest University, Xi'an 710069, China

*Email: wangy@mail.ipc.ac.cn

EXPERIMENTAL SECTION

Materials: TXO-PhCz was synthesized as reported previously. Poly(styrene sulfonic acid)-doped poly(3,4-ethylenedioxythiphene) (PEDOT:PSS, Baytron PVP A4083) was purchased from H.C. Starck GmbH. 1,1-bis[(di-4-tolylamino)phenyl] cyclohexane (TAPC), 1,3-bis[(4-tert-butylphenyl)-benzene (TmPyPB), and TPBI with a purity of more than 99% was purchased from Jilin Optical and Electronic Materials Company, which were purified by repeated temperature-gradient vacuum sublimation. LiF was purchased from Sigma-Aldrich.

Photophysical characterization: UV-vis spectra and fluorescence spectra were obtained with Hitachi U-3900 and F-4600 spectrophotometers, respectively. The absolute fluorescence quantum yields of the solid films are measured with an integrating sphere. The transient PL decay and temperature dependence of the TXO-PhCz:TPBI or TXO-PhCz:mCP films were measured using a Edinburgh Instruments FLS920 spectrometer. T_1, A_1, T_2, A_2 were obtained from the multi-exponential fitting of the transient decay curves on a 200 μs scale. The fit parameters is fit $=A_1 \exp(-t/\tau_1)+A_2 \exp(-t/\tau_2)$. Φ_p and Φ_d were determined by using total PL quantum efficiency and the ratio between prompt and delayed components which was calculated from transient PL measurements.

Device fabrication: OLEDs were fabricated on patterned ITO-coated glass substrates with a sheet resistance of 15 Ω/□. Before device fabrication, the ITO glass substrates were ultrasonically cleaned with detergent, de-ionized water, acetone, and alcohol. The substrates were dried in an oven at 120°C and then treated with UV-ozone for 10 mins.

A layer of 30 nm thick PEDOT:PSS was spin-coated onto the pre-cleaned substrate and bake in a glovebox under a nitrogen environment (oxygen and water contents less than 1 ppm) at 120°C for 30 mins to extract residual water. Afterward, the substrates were transferred into a vacuum deposition system with a base pressure lower than 1×10^{-6} mbar for organic semiconductor and metal deposition. The evaporation rate of organic semiconductors is about 1~2 Å/s, and the deposition rate of LiF is about 0.1 Å/s. The fabrication of OLEDs was finished by the Al electrode deposition with an evaporation rate of 10 Å/s. The thickness of evaporated films were monitored by frequency `counter, and calibrated by Dektak 6M Profiler. The EL luminescence spectra and CIE color coordinates were measured by a Spectra scan PR655 photometer. The current-voltage-brightness characteristics were measured by using a computer-controlled Keithley source measurement unit (Keithley 2400 Source Meter) with a calibrated optical power meter of Newport company (1936R) under ambient atmosphere. The hole-only device and the electron-only device were fabricated with the similar procedure above.

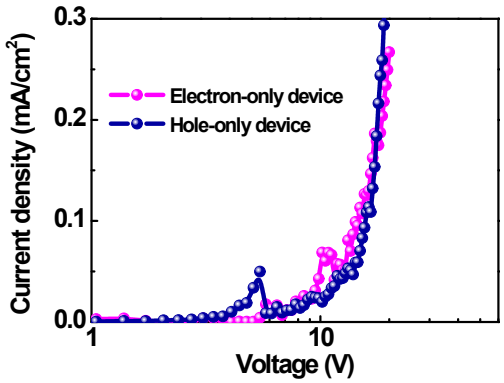

Fig. S1 The current density (*J*)-voltage (*V*) characteristics of single carrier transport devices. Hole-only device: ITO/PEDOT (40 nm)/TAPC (40 nm)/mCP (20 nm)/EML (30 nm)/WO_3 (10 nm)/Al (100 nm); Electron-only device: ITO/EML (30 nm)/TmPyPB (130 nm)/ LiF (1.8 nm)/Al (100 nm).

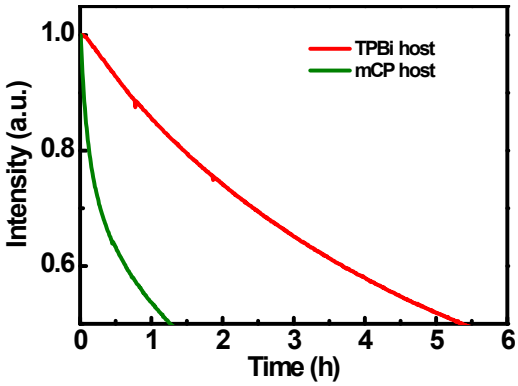

Fig. S2. The lifetime of the devices based on the TPBI and mCP host. The device structures: ITO/HAT-CN (10 nm)/TAPC (30 nm)/mCP (10 nm)/TPBi (mCP):5 wt% TXO-PhCz (30 nm)/TmPyPB (40 nm)/LiF (0.9 nm)/Al.