Supplementary information

Suppression of benzophenone-induced triplet quenching for enhanced TADF performance

Gediminas Kreiza[1], Dovydas Banevičius[1], Justina Jovaišaitė[1], Karolina Maleckaitė[1], Dalius Gudeika[2], Dmytro Volyniuk[2], Juozas V. Gražulevičius[2], Saulius Juršėnas[1], Karolis Kazlauskas[1]

[1]Institute of Photonics and Nanotechnology, Vilnius University, Saulėtekio av. 3, LT-10257 Vilnius, Lithuania
[2]Department of Polymer Chemistry and Technology, Kaunas University of Technology, Radvilenu pl. 19, LT- 50254, Kaunas, Lithuania

Experimental

^{1}H NMR (300 MHz) and ^{13}C NMR (75 MHz) spectra were recorded on a Varian Unity Inova 300 apparatus. IR spectra were recorded on a Perkin-Elmer Spectrum GX II FT-IR System spectrometer. Mass spectra were recorded on a Waters SQ Detector 2. Elemental analysis was performed with an Exeter Analytical CE-440 Elemental Analyzer. Differential scanning calorimetry (DSC) measurements were carried out using a DSC Q2000 calorimeter (TA Instruments) under nitrogen environment (scan rate 10 $^\circ$C/min). Thermogravimetric analysis (TGA) was performed on a TA Instruments Q50 apparatus under nitrogen gas (scan rate 20 $^\circ$C/min). Ionization potentials (IP) of the vacuum-deposited films were estimated by photoelectron emission spectrometry in air.[1] The measurements were carried out using a deep-UV deuterium light source ASBN-D130-CM, a CM110 1/8m monochromator, and an electrometer 6517B (Keithley). Charge carrier mobility (μ) measurements of several-micron-thick solid films of the studied compounds deposited on indium tin oxide (ITO) and covered by aluminum layer on top were performed by using the time-of-flight (TOF) method.[2] The pulsed laser (EKSPLA NL300, wavelength 355 nm, pulse duration 5 ns) was used as an excitation source in the TOF measurements. Hole and electron transport in the solid films at different electric fields was investigated by applying different positive and negative external voltages (U) to the samples utilizing electrometer 6517B (Keithley). Photocurrent transients of charge carriers were recorded by TDS 3032C oscilloscope (Tektronix). Drift mobility values

were deduced from a relationship $\mu = d^2/(U \times t_{tr})$, where t_{tr} is a charge carrier transit time, d is the film thickness and U is applied voltage at the moment of excitation.

Table S1. Absorption energies, oscillator strengths and singlet-triplet energy gap for 5tCzMeB and 5tCzBP calculated by TD-DFT B3LYP/6-31G(d) in vacuum.

Compound	$S_0 \to S_1$ (eV)	$f_{S0 \to S1}$	$S_0 \to T_1$ (eV)	ΔE_{ST} (eV)
5tCzMeB	3.04	0.0267	2.79	0.25
5tCzBP	2.69	0.0066	2.64	0.05
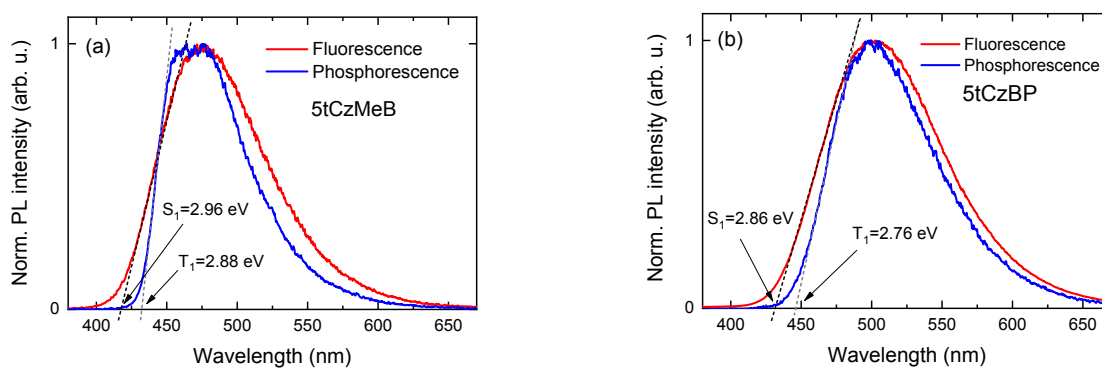
Figure S1. Room temperature fluorescence and phosphorescence (at 10 K) spectra of 5tCzMeB and 5tCzBP in PMMA films at 1 wt% doping. Phosphorescence spectra were obtained at a delay of 0.1 ms.
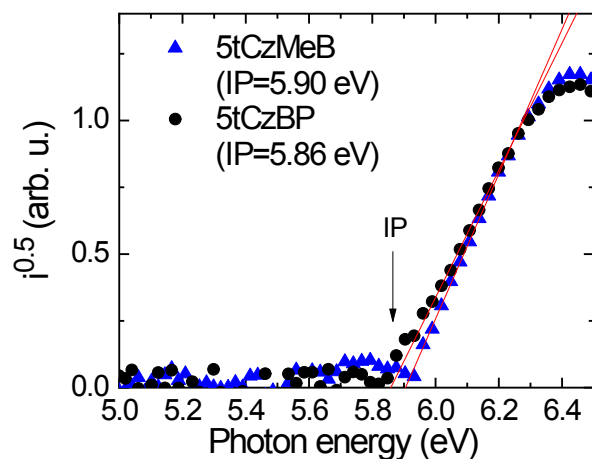
Figure S2. Determination of ionization potential in 5tCzMeB and 5tCzBP neat films by photoelectron emission spectroscopy.
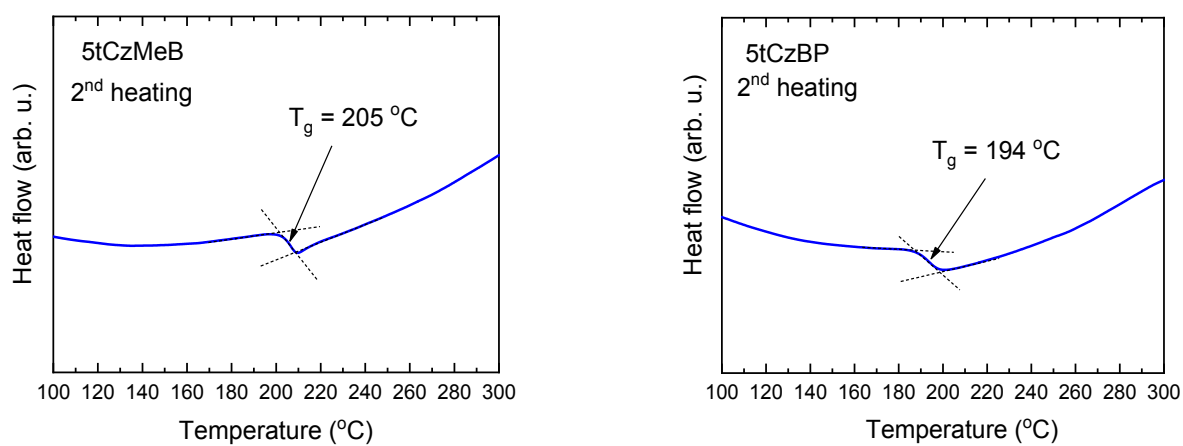

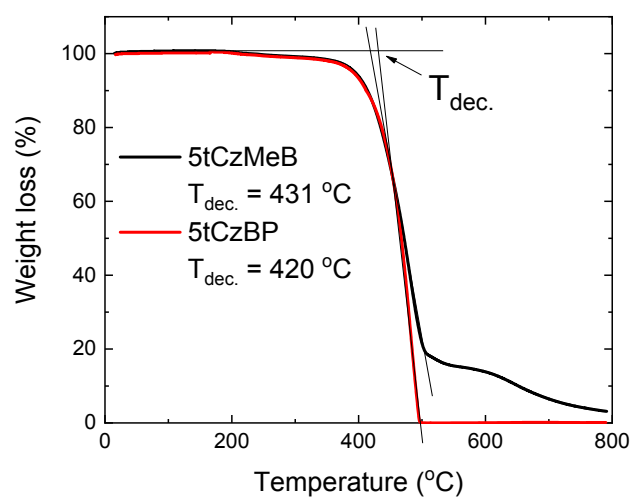**Figure S3.** DSC 2nd heating curves of 5tCzMeB and 5tCzBP compounds.

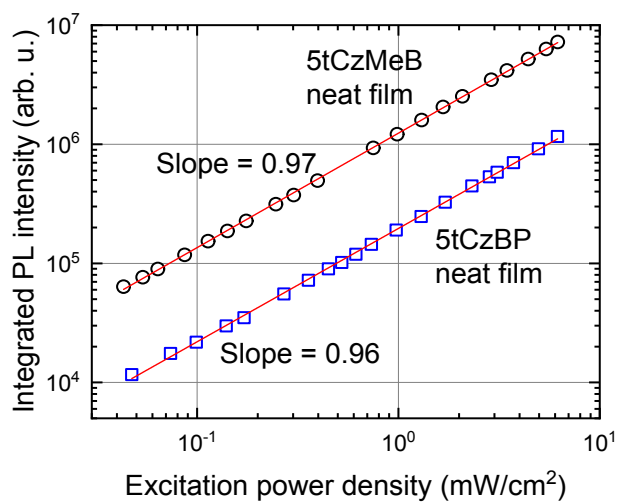**Figure S4.** TGA curves of 5tCzMeB and 5tCzBP with thermal degradation temperatures indicated.

Figure S5. PL intensity as a function of excitation power density in the neat films of 5tCzMeB and 5tCzBP. 375 nm CW laser diode was used as an excitation source.
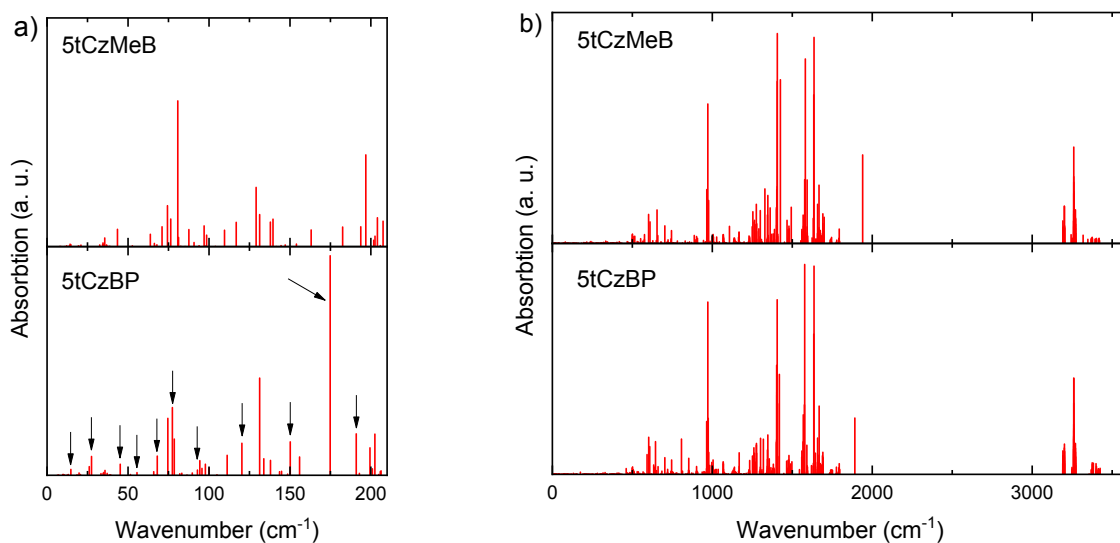
Figure S6. IR vibrational spectra of 5tCzMeB and 5tCzBP calculated in the ground state geometry by using HF/3-21G method. Low frequency modes associated with loose phenyl moiety of 5tCzBP are indicated by arrows.
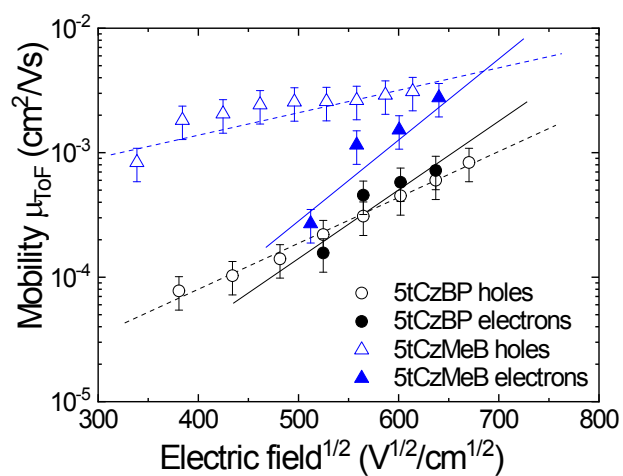

Figure S7. Electron and hole mobilities in solution-processed neat films of 5tCzBP and 5tCzMeB determined by TOF measurements.
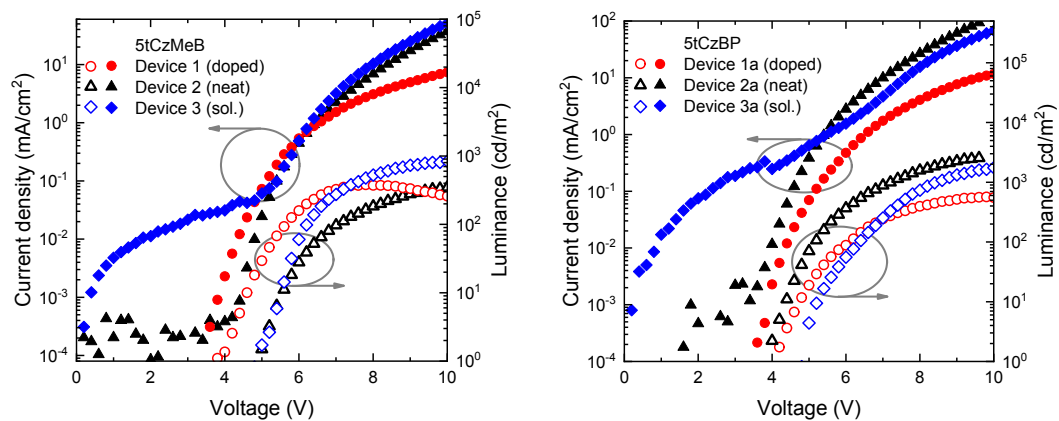
Figure S8. Semi-log plot of current density and luminance as a function of applied voltage of fabricated devices.

References

1   E. Miyamoto, Y. Yamaguchi and M. Yokoyama, *Electrophotography*, 1989, **28**, 364–370.

2   W. Warta and N. Karl, *Phys. Rev. B*, 1985, **32**, 1172–1182.