Supporting Information

Nondoped Deep-blue Spirofluorenexanthene-based Green Organic Semiconductors via a Pot, Atom and Step Economic (PASE) Route Combining Direct Arylation and Tandem Reactions

Ming-Li Sun [a], Wen-Sai Zhu [c], Zhen-Song Zhang [b], Chang-Jin Ou [a], Ling-Hai Xie [a,], Yang Yang [c], Yan Qian [a], Yi Zhao [b], Wei Huang [a,c,*]*

[a]*Center for Molecular Systems and Organic Devices (CMSOD), Key Laboratory for Organic Electronics & Information Displays (KLOEID) and Institute of Advanced Materials (IAM), Nanjing University of Posts & Telecommunications, Nanjing 210046, Jiangsu, China*

[b]*State Key Laboratory of Integrated Optoelectronics, College of Electronics Science and Engineering, Jilin University, Changchun 130012, Jilin, China*

[c]*Jiangsu-Singapore Joint Research Center for Organic/Bio-Electronics & Information Displays and Institute of Advanced Materials (IAM), Nanjing Tech University, Nanjing 211816, Jiangsu, China*

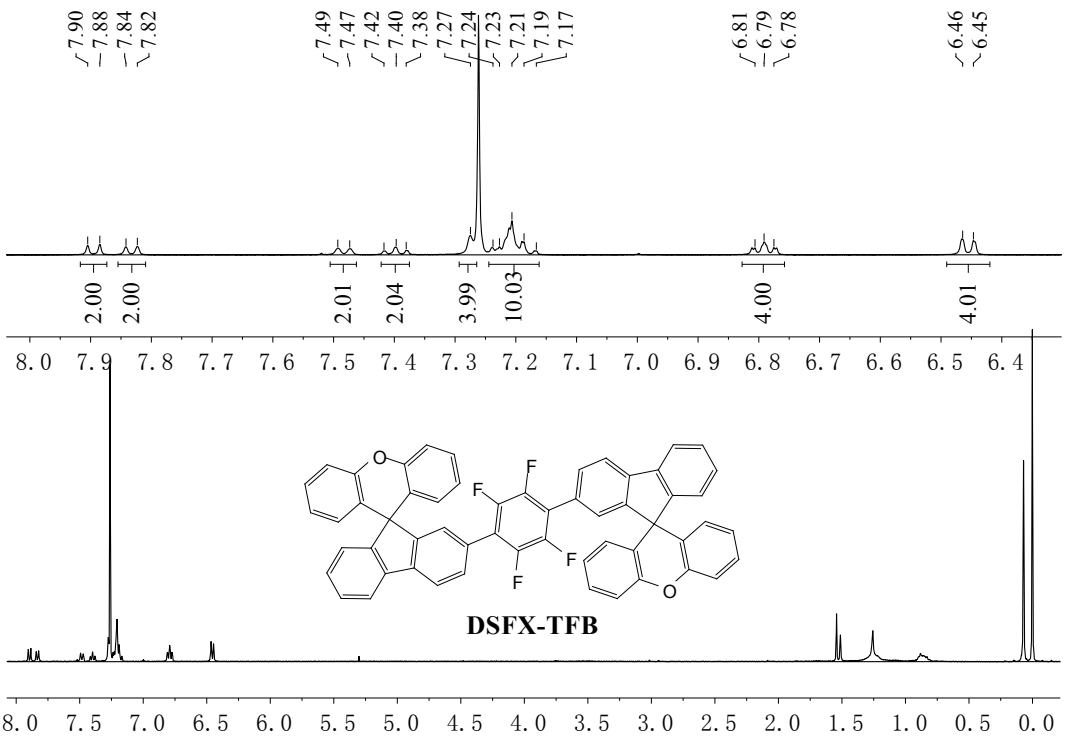
E-mail: wei-huang@njtech.edu.cn ; iamlhxie@njupt.edu.cn

Fax: +86 25 5813 9988; Tel: +86 25 5813 9001

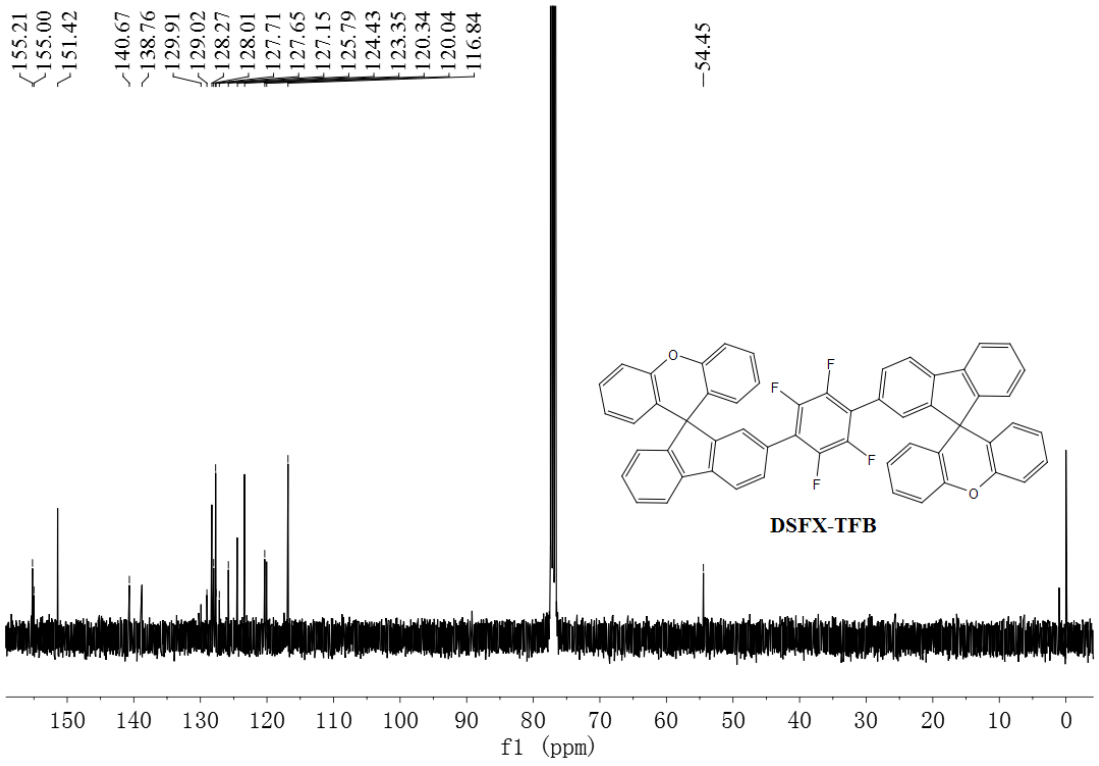
EXPERIMENTAL SECTION

Chemicals. All reagents were purchased from Sigma-Aldrich, Merck and Alfa Aesar, and used as received unless stated otherwise. Anhydrous THF (HPLC grade) was collected from Solvent Purification Systems (Innovative Technology, Inc.). Anhydrous chloroform was pre-dried over molecular sieves.

Characterization: ^{1}H-NMR in $CDCl_3$ was recorded at 400 MHz using a Varian Mercury 400 plus spectrometer. For the MALDI-TOF MS spectra, the spectra were recorded in reflective mode, no substrates were used. Elemental analyses were carried out on an Elementar Analysensysteme GmbH Vario EL *III* Instrument. Absorption spectra were measured with a Shimadzu UV-3150 spectrometer and emission spectra were recorded on a Shimadzu RF-530XPC luminescence spectrometer. Differential scanning calorimetry (DSC) analyses were performed on a Shimadzu DSC-60A Instrument. Thermogravimetric analyses (TGA) were conducted on a Shimadzu DTG-60H thermogravimetric Analyzer under a heating rate of 10°C/min and a nitrogen flow rate of 20 cm^3/min. Cyclic voltammetric (CV) studies were conducted using an CHI600C in a typical three-electrode cell with a platinum sheet working electrode, a platinum wire counter electrode, and a silver/silver nitrate (Ag/Ag^+) reference electrode.



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.89 (d, *J* = 8.0 Hz, 2H), 7.83 (d, *J* = 7.5 Hz, 2H), 7.48 (d, *J* = 7.9 Hz, 2H), 7.40 (t, *J* = 7.3 Hz, 2H), 7.27 (s, 4H), 7.24 – 7.16 (m, 10H), 6.79 (t, *J* = 6.2 Hz, 4H), 6.46 (d, *J* = 7.1 Hz, 4H).



^{13}C NMR (101 MHz, $CDCl_3$) δ 155.21 (s), 155.00 (s), 151.43 (s), 140.67 (s), 138.88 – 138.68 (m), 129.91 (s), 129.02 (s), 128.28 (s), 128.01 (s), 127.71 (s), 127.65 (s), 127.15 (s), 125.79 (s), 124.47 (s), 123.36 (s), 120.34 (s), 120.06 (s), 116.84 (s), 54.45 (s).

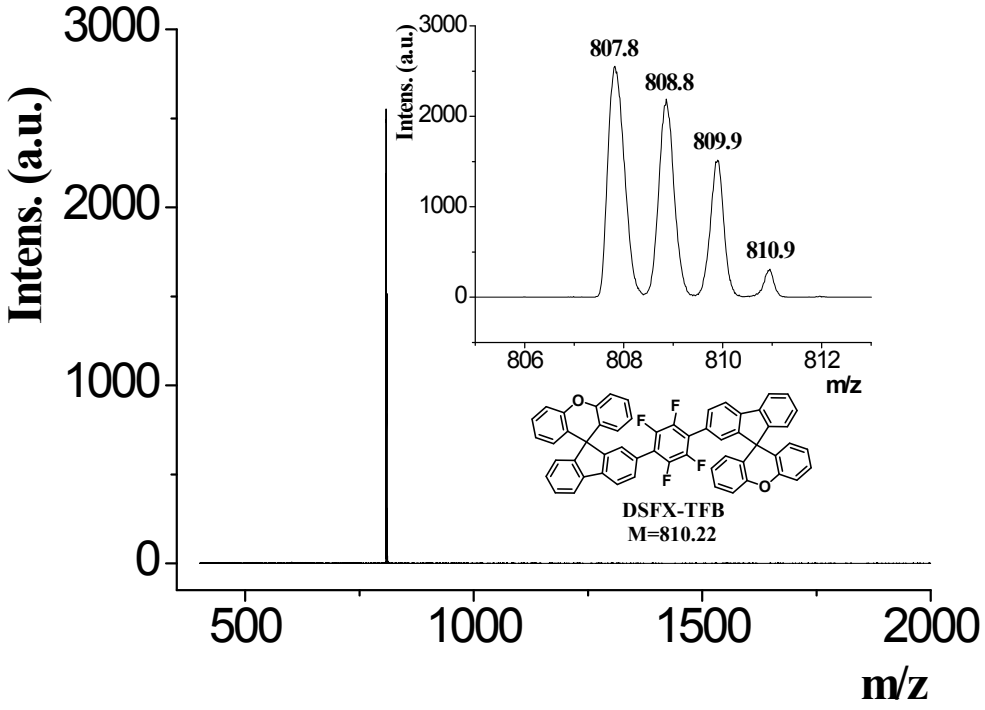


Figure S1. ^{1}H-NMR, ^{13}C-NMR and MALDI-TOF mass spectra of DSFX-TFB.

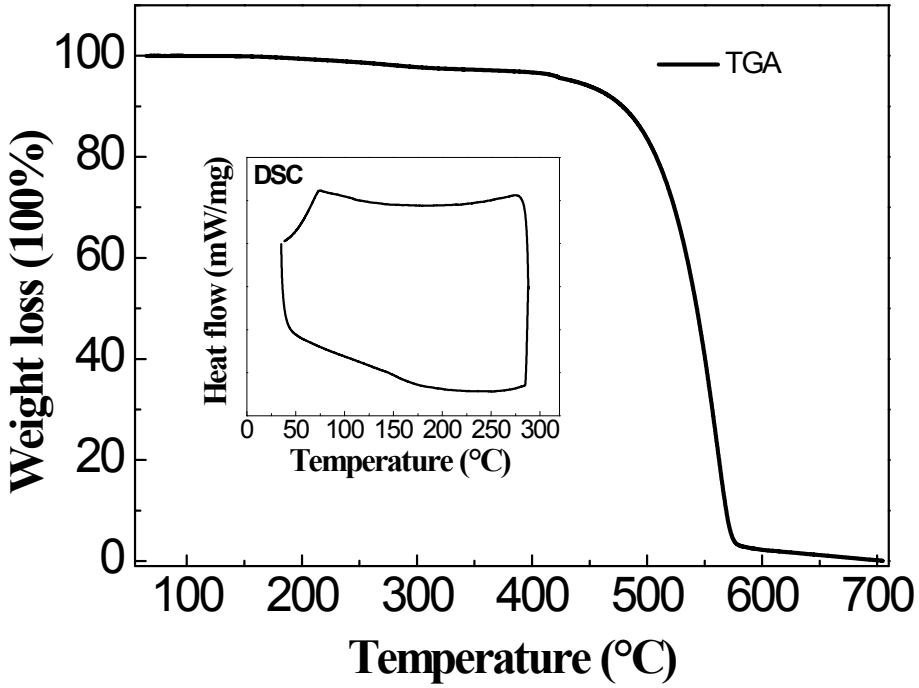
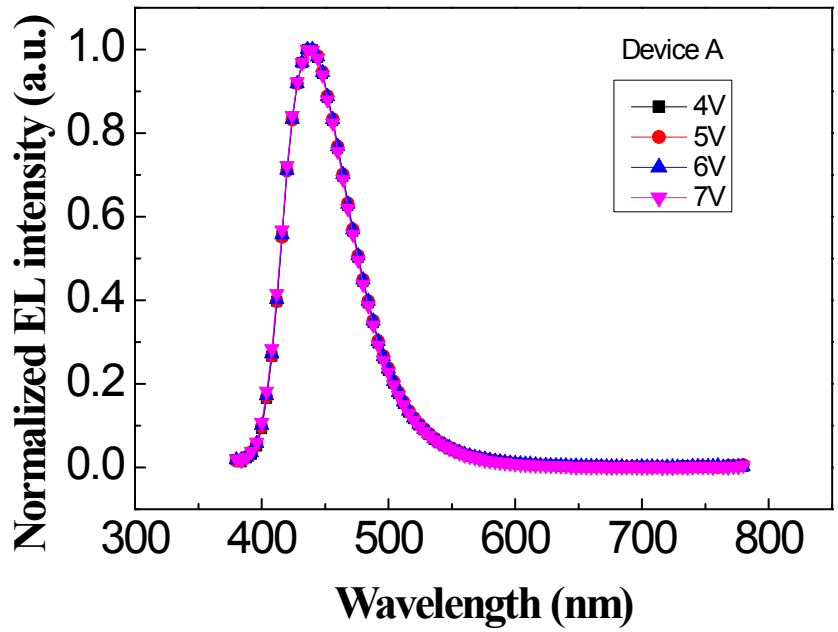
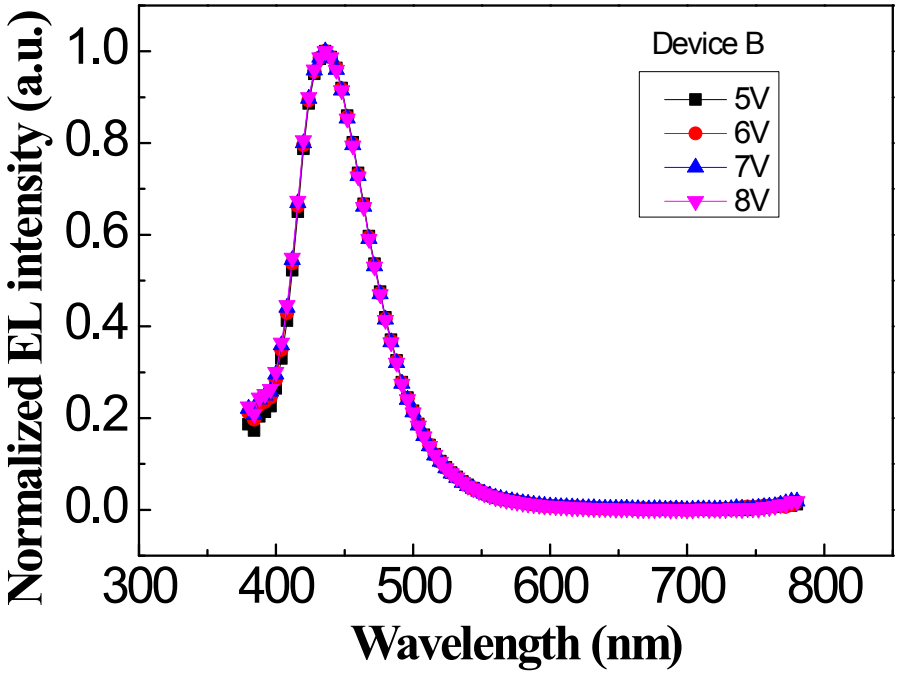
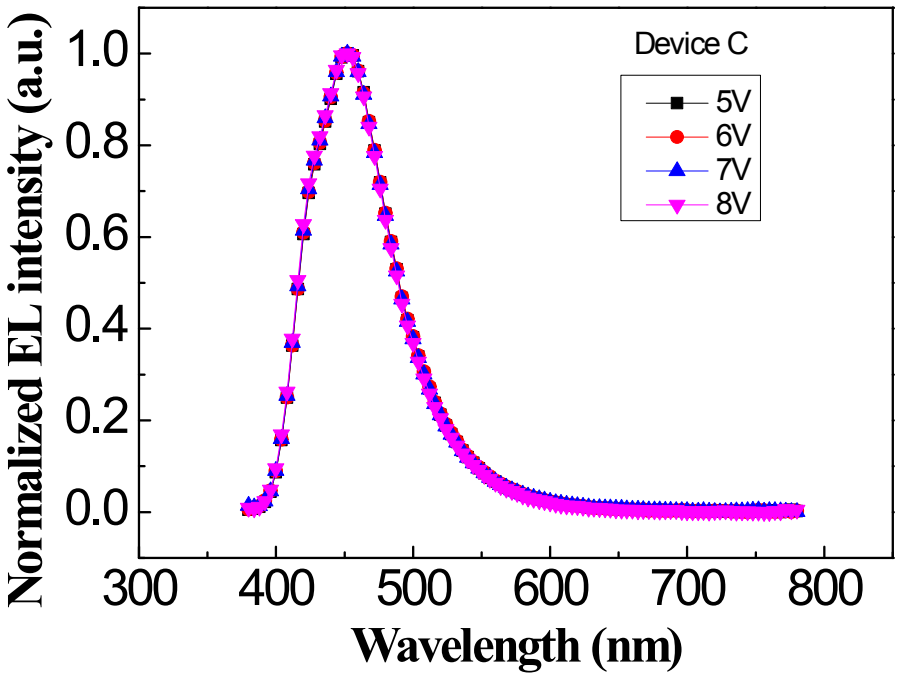
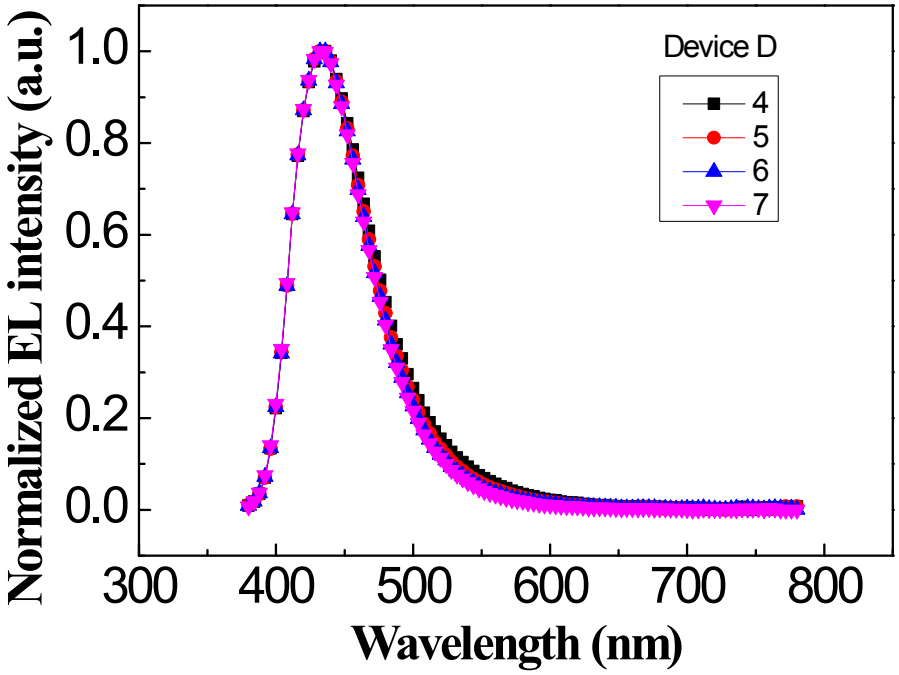


Figure S2. The TGA and DSC curve of DSFX-TFB.


Device A
4V
5V
6V
7V
Normalized EL intensity (a.u.)
1.0
0.8
0.6
0.4
0.2
0.0
300
400
500
600
700
800
Wavelength (nm)


Device B
5V
6V
7V
8V
Normalized EL intensity (a.u.)
1.0
0.8
0.6
0.4
0.2
0.0
300
400
500
600
700
800
Wavelength (nm)


Device C
5V
6V
7V
8V
Normalized EL intensity (a.u.)
1.0
0.8
0.6
0.4
0.2
0.0
300
400
500
600
700
800
Wavelength (nm)


Device D
4
5
6
7
Normalized EL intensity (a.u.)
1.0
0.8
0.6
0.4
0.2
0.0
300
400
500
600
700
800
Wavelength (nm)

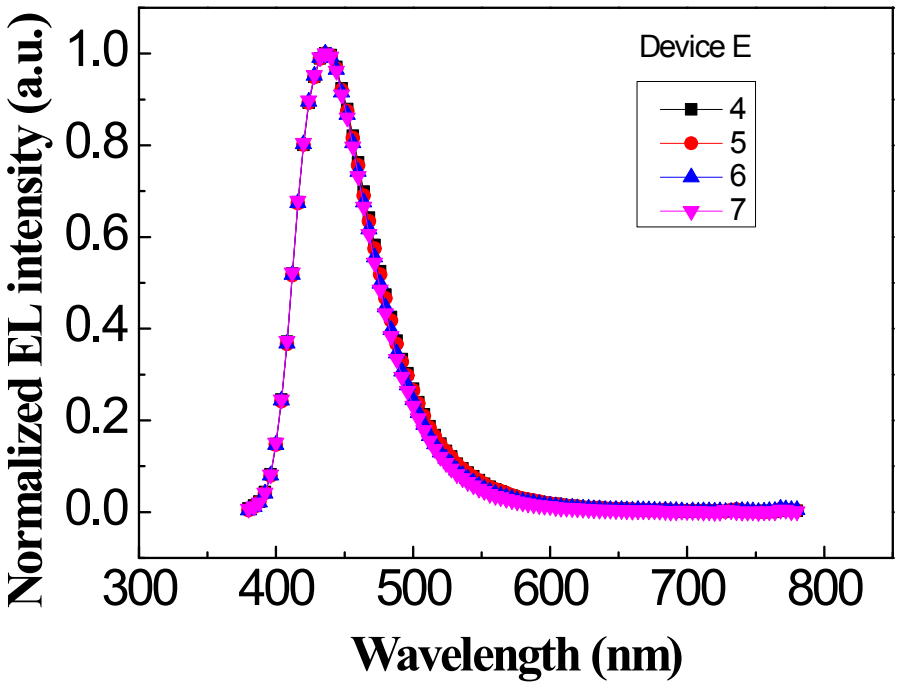
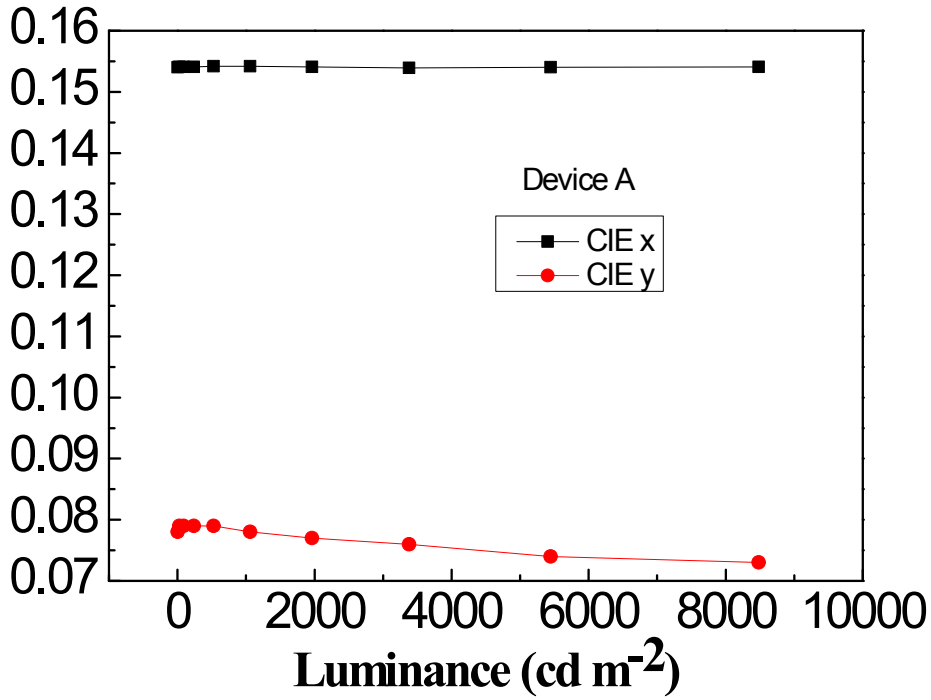
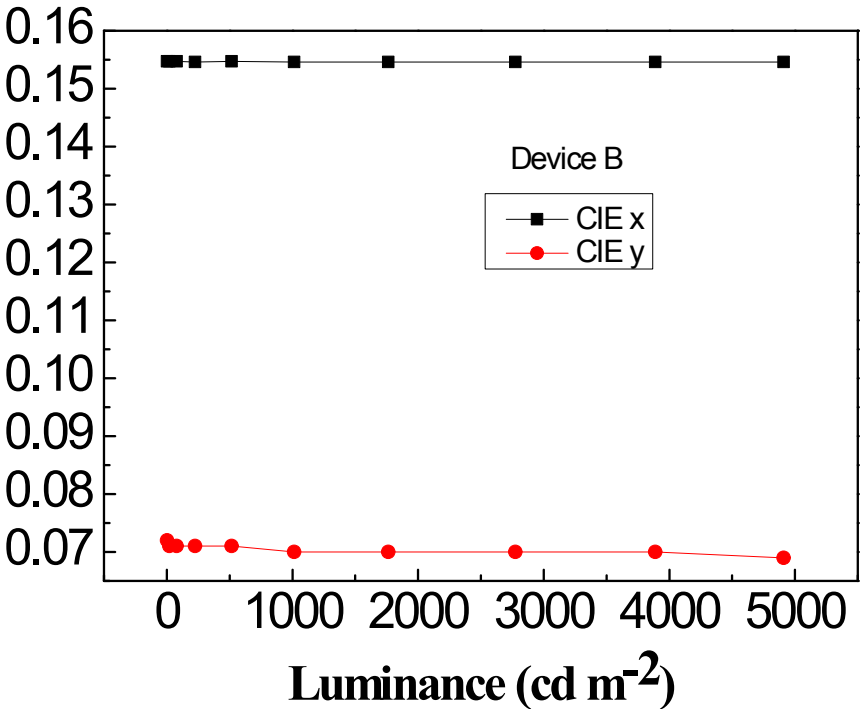
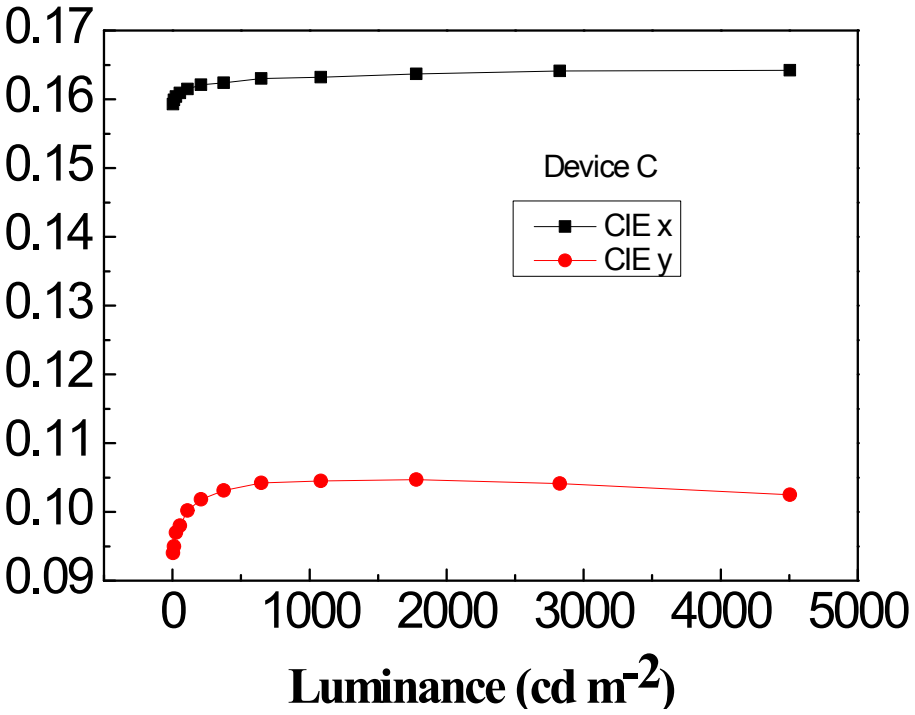
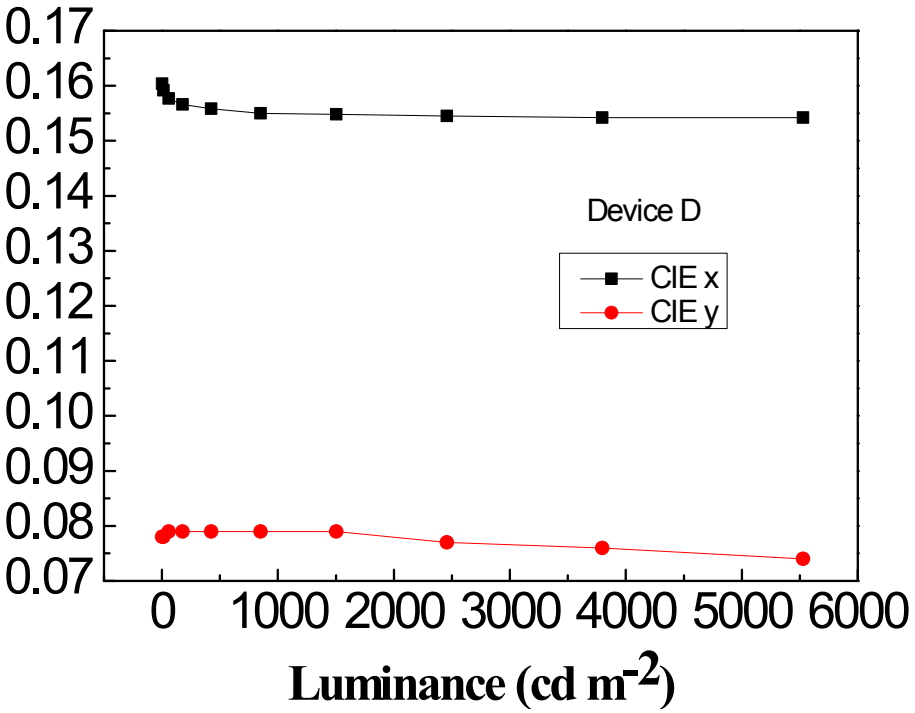


Figure S3. Normalized EL spectra of device A-E at the different Voltage.




0.16
0.15
0.14
0.13
0.12
0.11
0.10
0.09
0.08
0.07
Device B
CIE x
CIE y
0
1000
2000
3000
4000
5000
Luminance (cd m-2)


0.17
0.16
0.15
0.14
0.13
0.12
0.11
0.10
0.09
Device C
CIE x
CIE y
0
1000
2000
3000
4000
5000
Luminance (cd m-2)



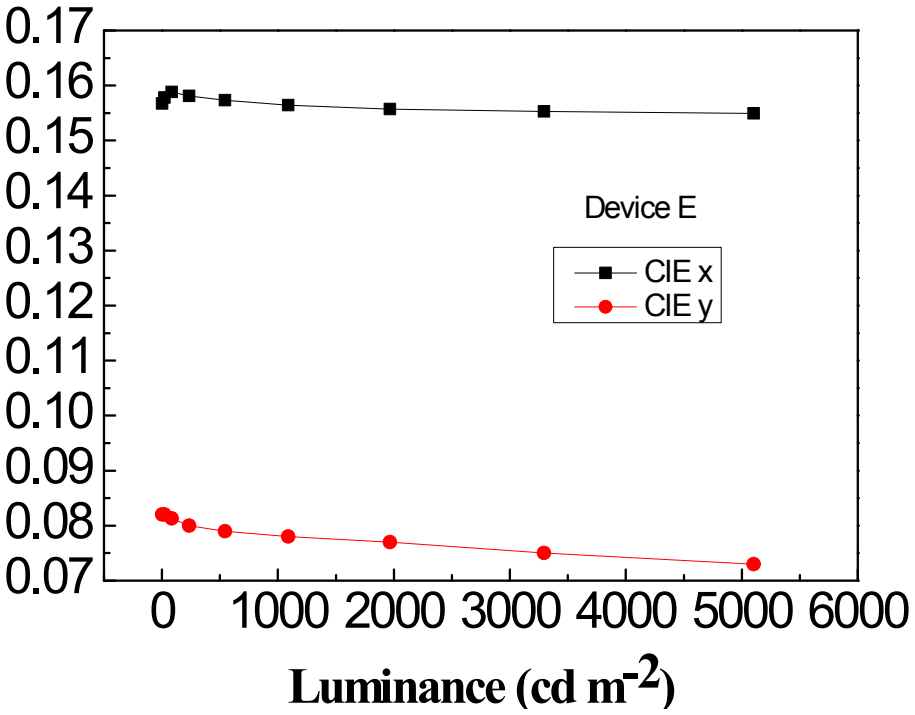


Figure S4. The CIE coordinates versus the voltage of the device A–E.

Table S1. Thermal and photophysical properties of the DSFX-TFB.

Cmpd.	$\lambda^{abs.}{}_{max}$ [a] (nm)	$\lambda^{em.}{}_{max}$ (FWHM) [b] (nm)	Φ [c]	T_d / T_g [d] (°C)	HOMO/ LUMO/Bandgap [e] (eV)
DSFX-TFB	322/330	375 (54)/401 (54)	0.81/0.66	440/ NA	-5.76/-2.39/ 3.37

[a] Maximum absorption measured in chloroform solution and solid film(vacuum deposited on quartz substrates). [b] Maximum emission wavelength and FWHM measured in solution and film. [c] Fluorescence quantum yields in solution/film, using 9,10-diphenyl-anthracence (Φ_{366} = 0.9) as a standard. [d] T_d: decomposition temperature, measured by TGA; T_g: glass transition temperature, measured by DSC. [e] HOMO and LUMO energy levels determined by cyclic voltammetry. NA: not available.