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

Supporting information

Novel phosphine oxide-based electron-transporting materials for efficient phosphorescent organic light-emitting diodes

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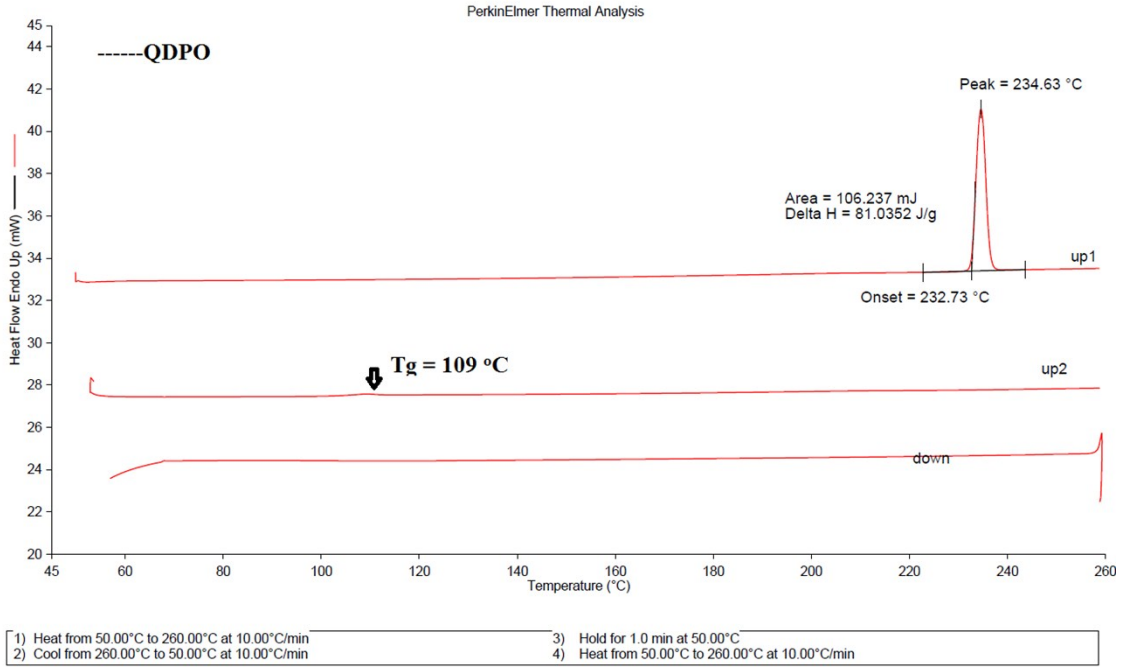
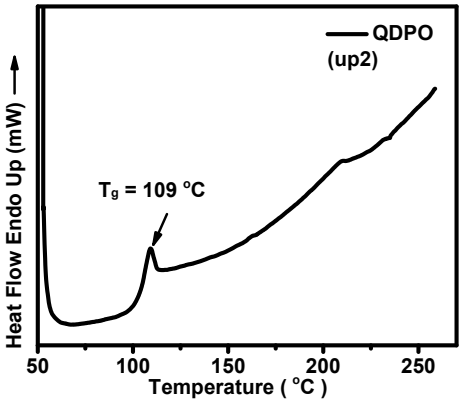
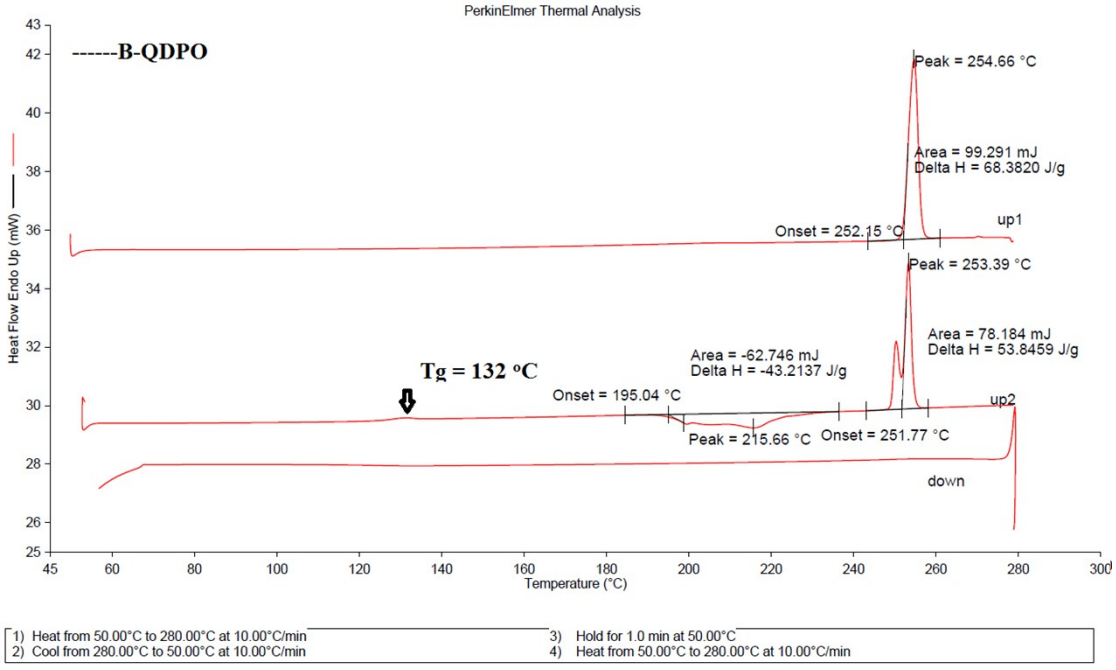
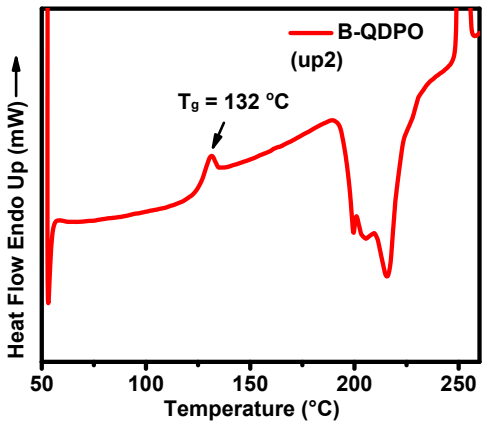



QDPO
(up2)
Tg = 109 °C
Heat Flow Endo Up (mW)
50
100
150
200
250
Temperature (°C)


PerkinElmer Thermal Analysis
------B-QDPO
Peak = 254.66 °C
Area = 99.291 mJ
Delta H = 68.3820 J/g
Onset = 252.15 °C
up1
Peak = 253.39 °C
Area = 78.184 mJ
Delta H = 53.8459 J/g
Tg = 132 °C
Area = -62.746 mJ
Delta H = -43.2137 J/g
Onset = 195.04 °C
up2
Peak = 215.66 °C
Onset = 251.77 °C
down
Heat Flow Endo Up (mW)
Temperature (°C)
1) Heat from 50.00°C to 280.00°C at 10.00°C/min
2) Cool from 280.00°C to 50.00°C at 10.00°C/min
3) Hold for 1.0 min at 50.00°C
4) Heat from 50.00°C to 280.00°C at 10.00°C/min


B-QDPO
(up2)
Tg = 132 °C
Heat Flow Endo Up (mW)
50
100
150
200
250
Temperature (°C)

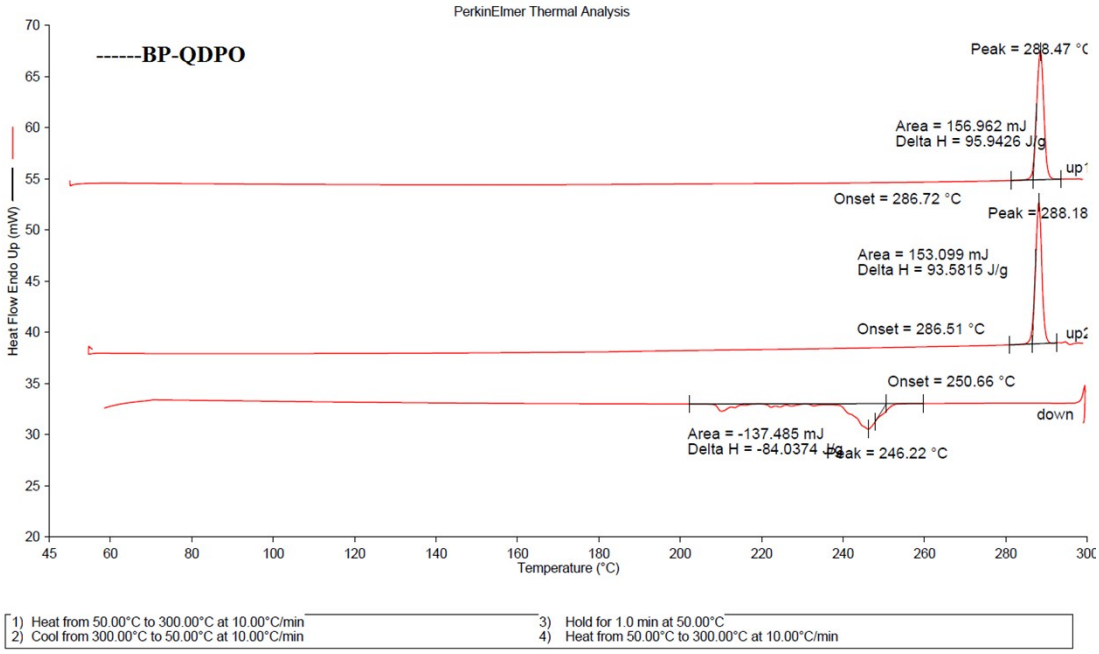


Fig. S1 DSC traces of **QDPO**, **B-QDPO** and **BP-QDPO** recorded at a heating rate of 10 ^{o}C min^{-1}.

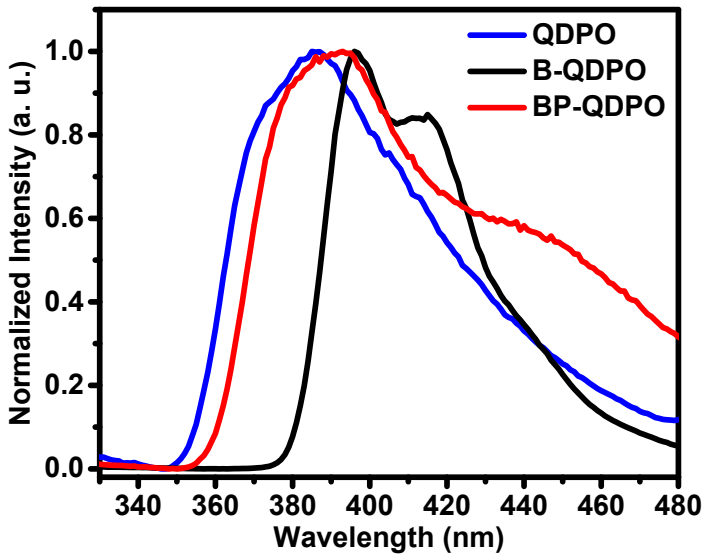


Fig. S2 The low temperature phosphorescence spectra of **QDPO**, **B-QDPO** and **BP-QDPO** at 77 K in in CH_2Cl_2 (10^{-5} M).

Table S1. The relevant data values for HOMO/LUMO levels of QDPO, B-QDPO and BP-QDPO.

Compound	$\Delta E_{ox\text{-}Ferrocene}$ [eV]	$\Delta E_{ox\text{-}complexes}$ [eV]	HOMO [eV]	λ_{ab} [nm]	E_g [eV]	LUMO [eV]
QDPO	**0.17**	**1.73**	**-6.36**	**350**	**3.54**	**-2.82**
B-QDPO	**0.17**	**1.56**	**-6.19**	**379**	**3.27**	**-2.92**
BP-QDPO	**0.17**	**1.48**	**-6.11**	**357**	**3.47**	**-2.64**
TPBi	0.17	1.44	-6.07	355	3.49	-2.58

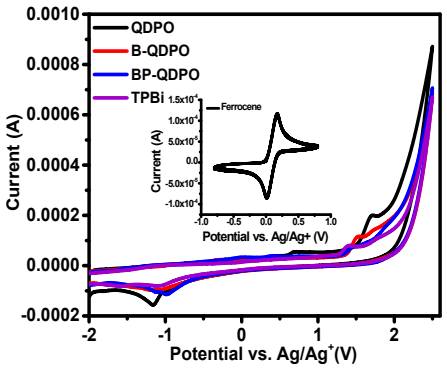
HOMO according to the peak of CV curves, $E_{HOMO} = E_{ox} - E^{+}_{Fc/Fc} + 4.8$; $E_{LUMO} = E_{HOMO} - E_g$; initial absorption spectra of QDPO, B-QDPO, BP-QDPO for E_g.

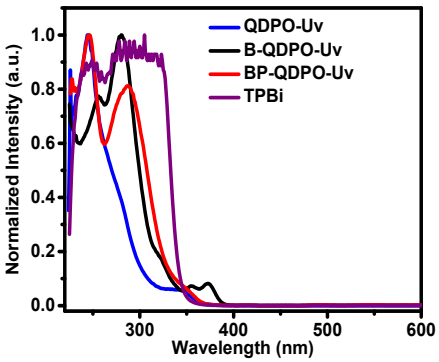
Example For QDPO:

$E_{HOMO} = E_{ox} - E^{+}_{Fc/Fc} + 4.8 = 1.73 - 0.17 + 4.8 = 6.36$ eV;

$E_g = 1240/350 = 3.54$ eV;

$E_{LUMO} = E_{HOMO} - E_g = 6.36\text{-}3.54 = 2.82$ eV.





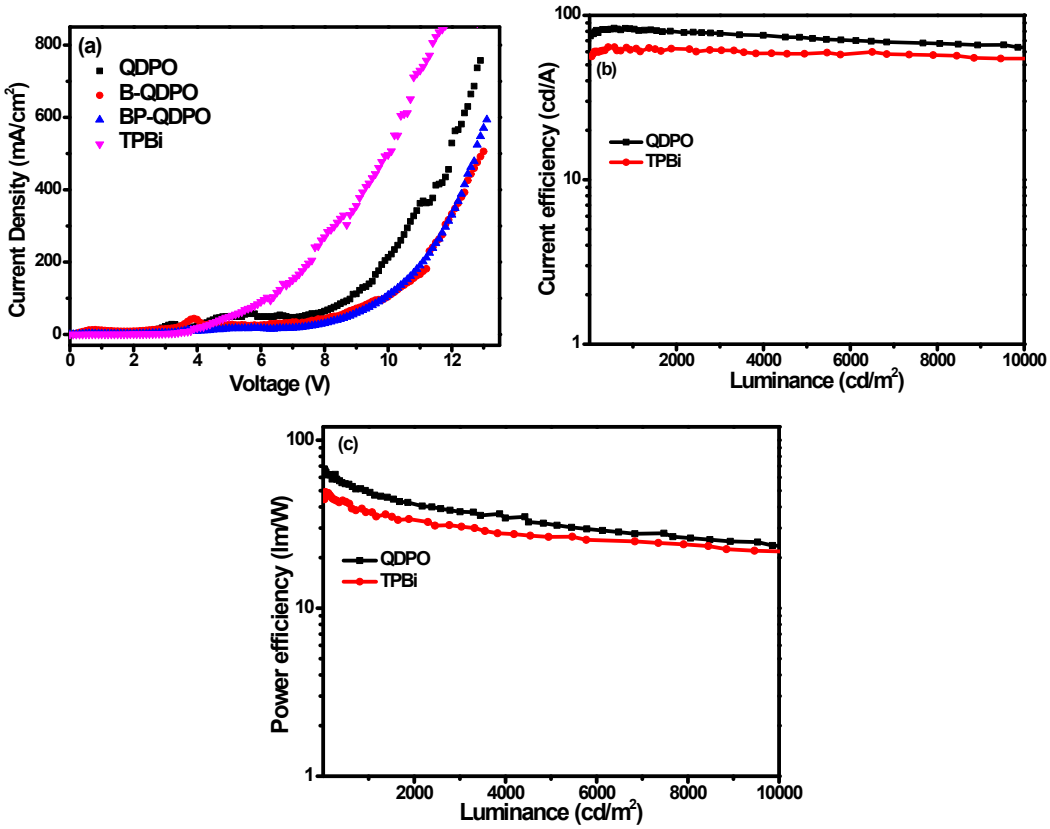
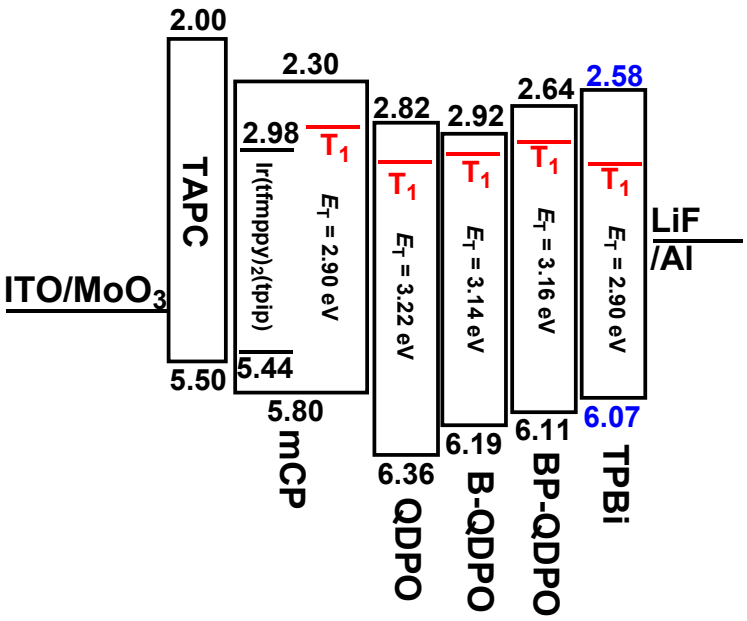


Fig. S3 (a) Current density versus voltage characteristics of the electron-only devices with the configuration of ITO/ TmPyPB (1,3,5-tri(m-pyrid-3-yl-phenyl) benzene, 60 nm)/QDPO, B-QDPO, BP-QDPO or TPBi (30 nm) /LiF (1 nm)/Al (100 nm); (b) and (c) EL performances of devices based on QDPO and TPBi.



E_T for QDPO = 3.22 eV, T_1 = -(6.36-3.22) = -3.14 ev
E_T for B-QDPO = 3.14 eV, T_1 = -(6.19-3.14) = -3.05 eV
E_T for BP-QDPO = 3.16 eV, T_1 = -(6.11-3.16) = -2.95 eV
E_T for TPBi = 2.90 eV, T_1 = -(6.07-2.90) = -3.17 eV
E_T for mCP = 2.90 eV, T_1 = -(5.80-2.90) = -2.90 eV

Fig. S4 The chemical structures of the used materials as well as the energy level diagram of the device architecture.