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Supporting information

Systematic tuning the ΔE_{ST} and charge balance property of the bipolar host for low operating voltage and high power efficiency solution-processed electrophosphorescent devices

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Content

To determine the change in dipole moment upon excitation, we used the Lippert-Mataga equation Eq. (1), which expressed the Stokes shift as a function of the solvent polarity parameter Δf(ε, n).

$$\Delta\nu = \nu_{abs} - \nu_f \cong \frac{2(\Delta\mu)^2}{hca^3}\Delta f(\varepsilon,n) + A \quad (1)$$

and Δf(ε, n) is calculated by

$$\Delta f(\varepsilon,n) = \frac{\varepsilon - 1}{2\varepsilon + 1} - \frac{n^2 - 1}{2n^2 + 1} \quad (2)$$

Here, $\Delta v = v_{abs} - v_f$ corresponds to the Stokes shift (in cm^{-1}) between the maxima of absorption and fluorescence emission. Fig S1 shows the PL emission in different solvents. The other terms: h, c and a respectively represent the Planck's constant, the velocity of light and the solute cavity radius.[39] In Eq. (2), n and ε are refractive index and the static dielectric constant of the solvent, respectively. Table S1 and S2 list the Δv values for xCz-PBI and Cz-nPBI in different solvents. Fig. S2 shows the linear Lippert-Mataga plots with the slope values of 16124, 13186, 10626, 8263, 8075 and 6567 cm^{-1} for 6Cz-PBI, 4Cz-PBI, 2Cz-PBI, Cz-2PBI, Cz-4PBI and Cz-6PBI, respectively.

Table S1 Spectral properties of xCz-PBI in different solvents

Solvents	$\Delta f(\varepsilon,n)$	2Cz-PBI			4Cz-PBI			6Cz-PBI		
		λ_{abs}(nm)	λ_f(nm)	ΔV(cm^{-1})	λ_{abs}(nm)	λ_f(nm)	ΔV(cm^{-1})	λ_{abs}(nm)	λ_f(nm)	ΔV(cm^{-1})
N-hexane	0.001	342	393	3794	349	433	5560	346	410	4511
Tetrahydrofuran	0.210	342	419	5373	347	468	7451	345	470	7709
Dichloromethane	0.218	344	435	6081	348	484	8074	347	476	7810
Ethanol	0.289	341	454	7299	346	511	9332	346	506	9138

Table S2 Spectral properties of Cz-nPBI in different solvents

Solvents	$\Delta f(\varepsilon,n)$	Cz-2PBI			Cz-4PBI			Cz-6PBI		
		λ_{abs}(nm)	λ_f(nm)	ΔV(cm^{-1})	λ_{abs}(nm)	λ_f(nm)	ΔV(cm^{-1})	λ_{abs}(nm)	λ_f(nm)	ΔV(cm^{-1})
N-hexane	0.001	299	390	7804	304	390	7250	305	379	6401
Tetrahydrofuran	0.210	297	403	8856	304	399	7832	304	401	7957
Dichloromethane	0.218	297	407	9100	301	404	8470	304	402	8019
Ethanol	0.289	297	421	9917	301	415	9126	303	413	8790

[a] Δf is the orientation polarizability parameter of the solvent. [b] λ_{abs} is absorption wavelength. [c] λ_{abs} is fluorescent wavelength. [d] ΔV is the Stokes shift between the maxima of absorption and fluorescence emission.

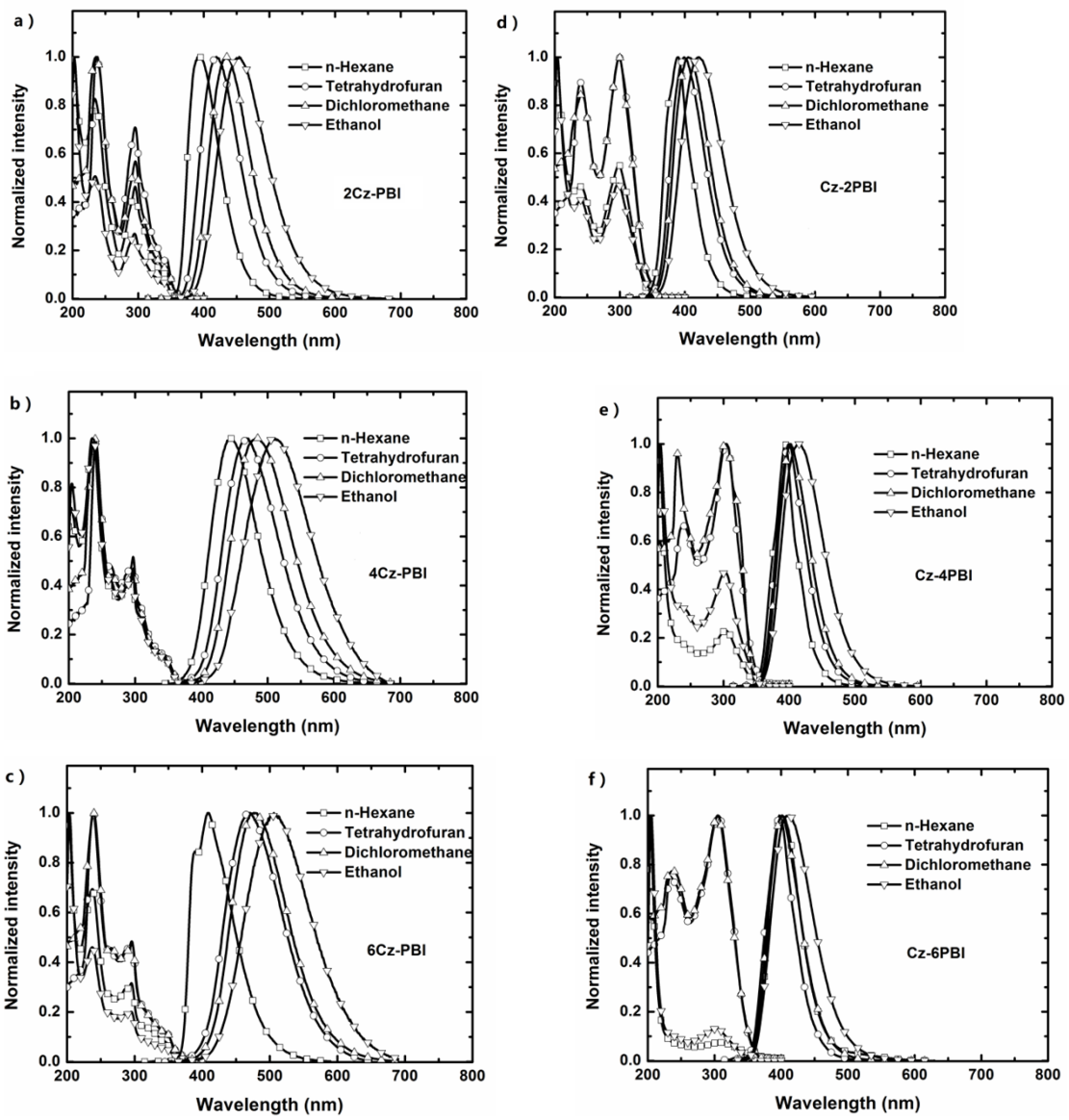

Figure S1. PL emissions of xCz-nPBI in different solvents.

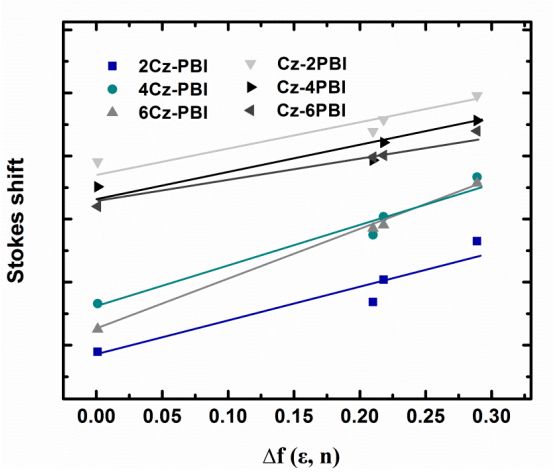

Figure S2. Lippert-Mataga plots of xCz-nPBI in various solutions.

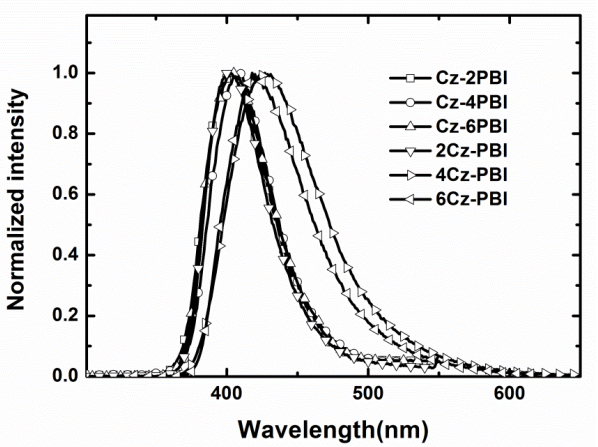

Figure S3. PL Emissions of xCz-nPBI in Film

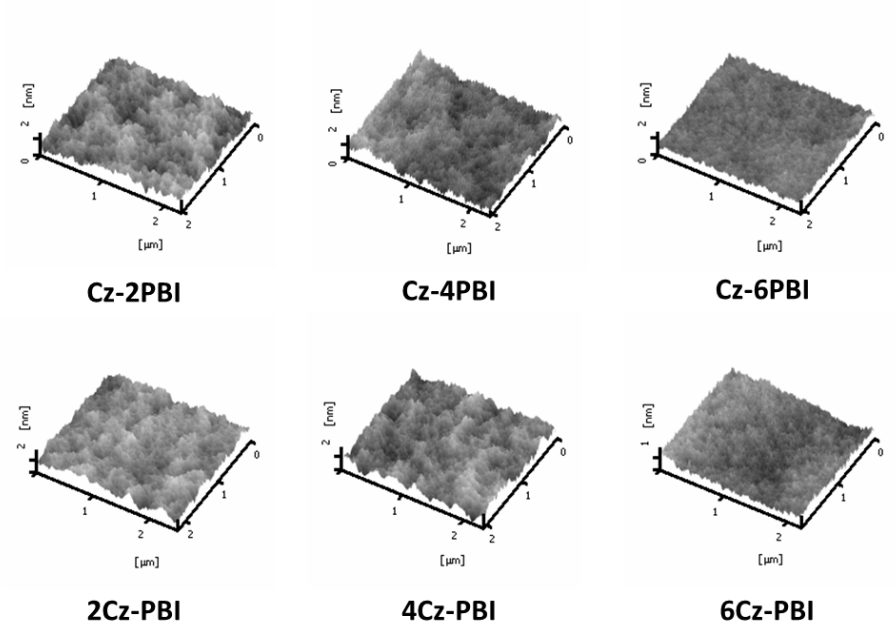

Figure S4. AFM Images of xCz-nPBI