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

Supporting Information

Impact of molecular structure on singlet and triplet exciton diffusion in phenanthroline derivatives

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Table S1: XRR fit parameters for thin films of phenanthroline derivatives

Layer	XRR Thickness (nm)	ρ (nm^{-3})	σ_R (nm)	Ellipsometer Thickness (nm)	ρ (Lit.) (nm^{-3})
Si		50	0-0.4		50 [1]
SiO_2	1-3	22.0	1-3	1.5	20.7-22.5 [1]
BPhen	16.2	2.26	1.1	15.4	2.27 ± 0.02 [2]
$BPhenCl_2$	20.8	2.04	1.2	20.5	
BCP	16.1	1.87	1.2	15.8	1.87 ± 0.02 [2]

X-ray reflectivity (XRR) is measured on a 20-nm-thick film of the active material deposited on a Si substrate using a PANalytical X'pert Pro instrument. The experimental data is simulated using GenX software to obtain thin film molecular density (ρ), surface roughness (σ_R) and film thickness.

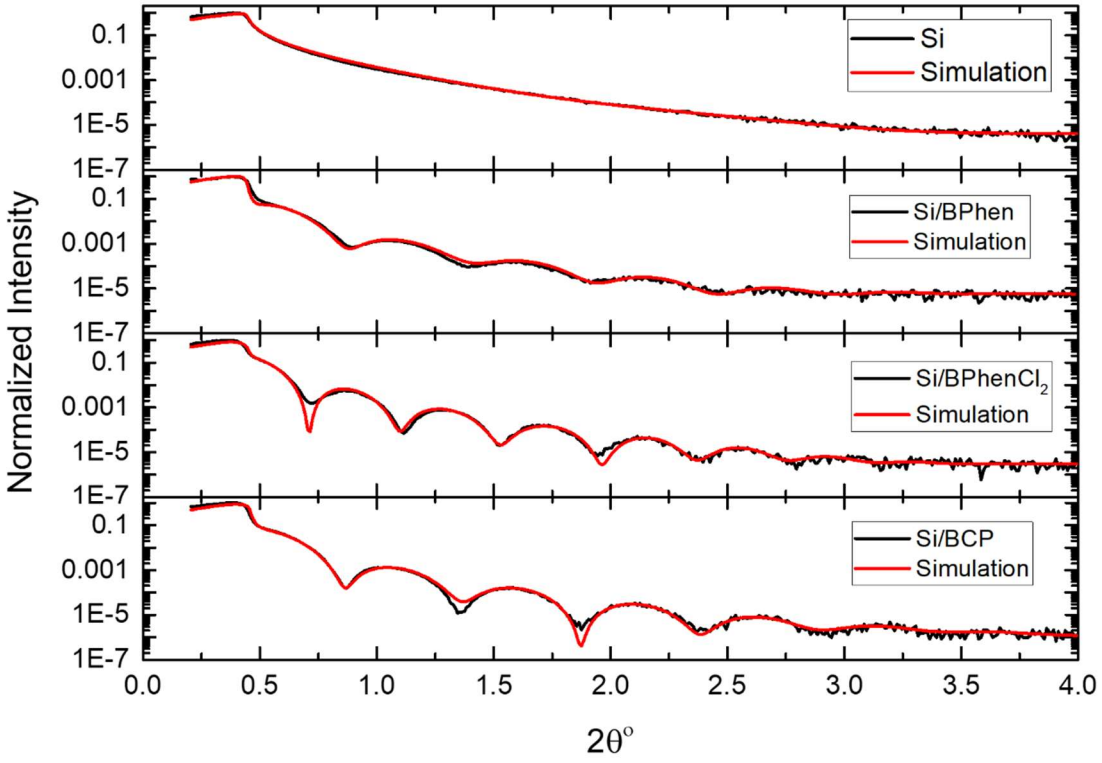

Figure S1: X-ray reflectivity on 20-nm-thick films (on a Si substrate) of BPhen, BPhen-Cl_2 and BCP. Data analysis is performed using GenX software with film thickness, density and roughness as fitting parameters. The extracted film thicknesses are within 5% of the values extracted from ellipsometry. The film roughness obtained from the fit is about 1.2 nm which is in close agreement with roughness value (RMS < 0.7 nm) obtained using atomic force microscopy (AFM).

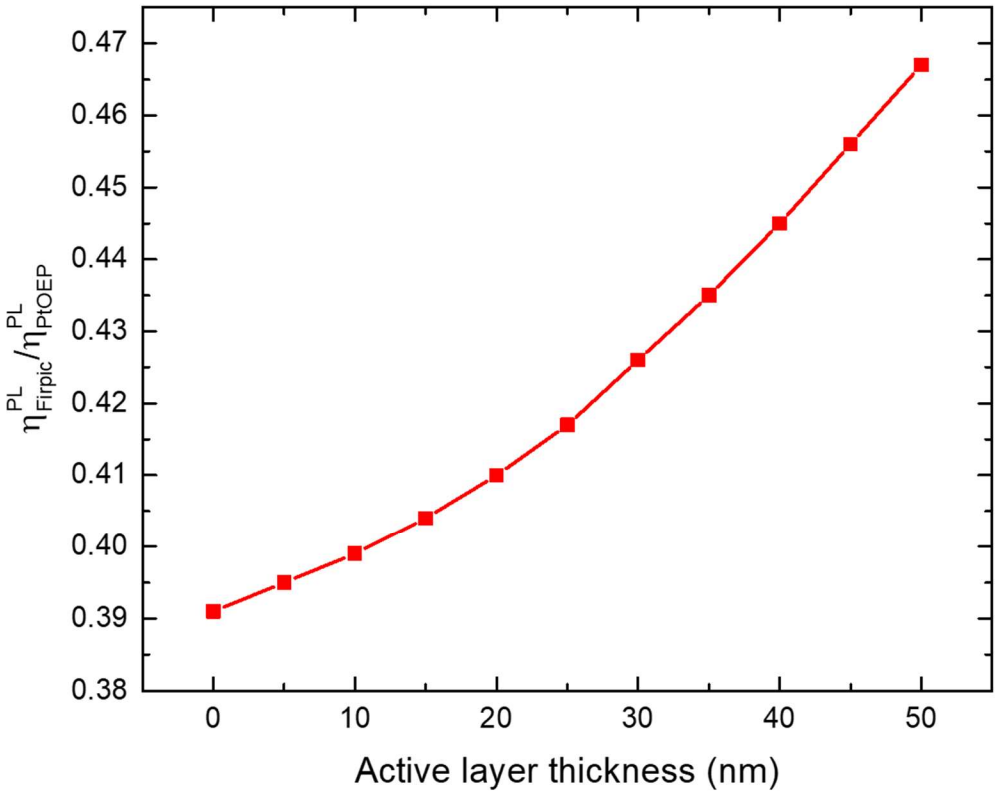

Figure S2: The simulated outcoupled photoluminescence efficiency ratio of FIrpic and PtOEP as a function of active layer thickness using Setfos 4.6 (Fluxim) software. The structure is simulated for FIrpic/active layer (x nm)/5 wt.% PtOEP, where the active layer is BPhen and its derivatives. The outcoupled photoluminescence efficiency ratios are same for all the three active layers due to similarity in optical constants.

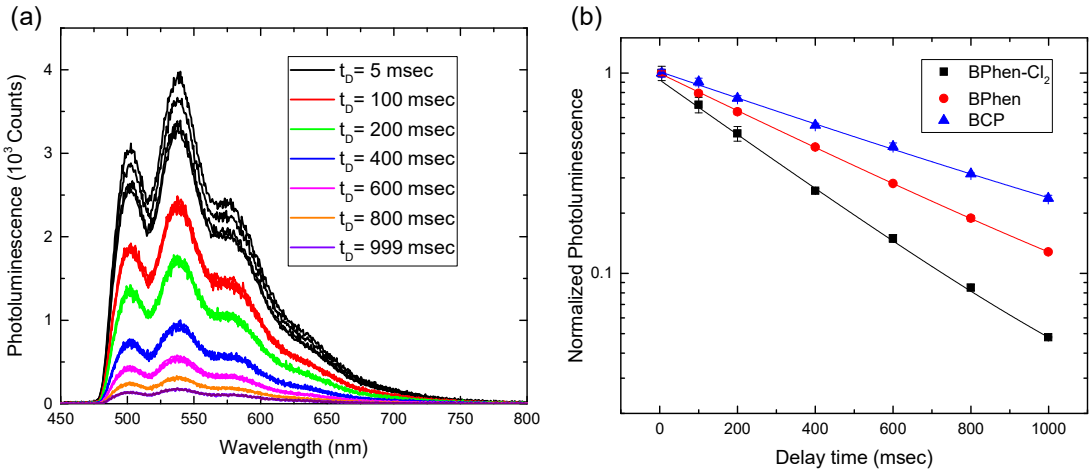

Figure S3: (a) Representative photoluminescence from the triplet state of BPhen-Cl_2 collected for different delay times from the trigger of a N_2 laser pulse at a wavelength of λ = 337 nm. (b) A semi-log plot between integrated photoluminescence from triplet state and delay times for phenanthroline derivatives.

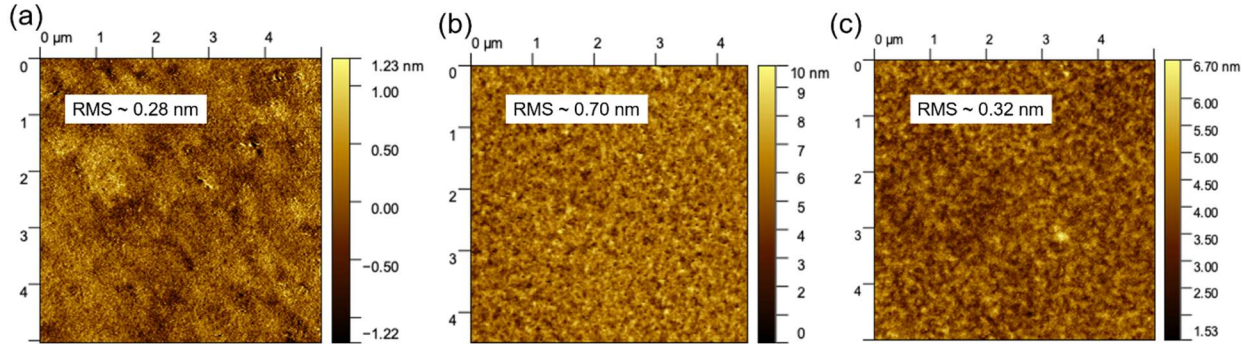

Figure S4: Atomic force micrographs of 30-nm-thick film of (a) BPhen (b) BPhen-Cl_2 and (c) BCP on a glass substrate. Atomic force microscopy was conducted using a Bruker Nanoscope V with a Multimode 8. Images were acquired in peak force quantitative nanomechanical (PF-QNM) mode, and AFM cantilevers were aluminum-coated n-type silicon with a nominal force constant of 0.6 N/m (HQ:NSC36/AL BS).

REFERENCES

1. Awaji; N., Sugita; Y., Nakanishi; T., Ohkubo; S., Takasaki; K., Komiya; S., High-precision x-ray reflectivity study of ultrathin SiO2 on Si, J. Vac. Sci. Technol, **1996**, A 14, 971.
2. Xiang, H. F.; Xu, Z. X.; Roy, V. A. L.; Che, C. M.; & Lai, P. T., Method for measurement of the density of thin films of small organic molecules, *Rev. Sci. Instrum.*, **2007,** 78, 034104.