

Supporting Information

N,N'-substituted Quinacridones for Organic Electronic Devices Applications

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Steady-state Photoluminescence Spectra of N,N' -Substituted Quinacridone Thin Films

For a qualitative comparison of the spectral shapes of the PL spectra in the low-energy regions, the normalized PL spectra measured for the three investigated materials in DMSO solution and thin films are shown in **Figure S1**. For better comparability, the normalized spectra measured for the DMSO solutions are shifted to match the position and relative intensities of the second vibronic PL peak.

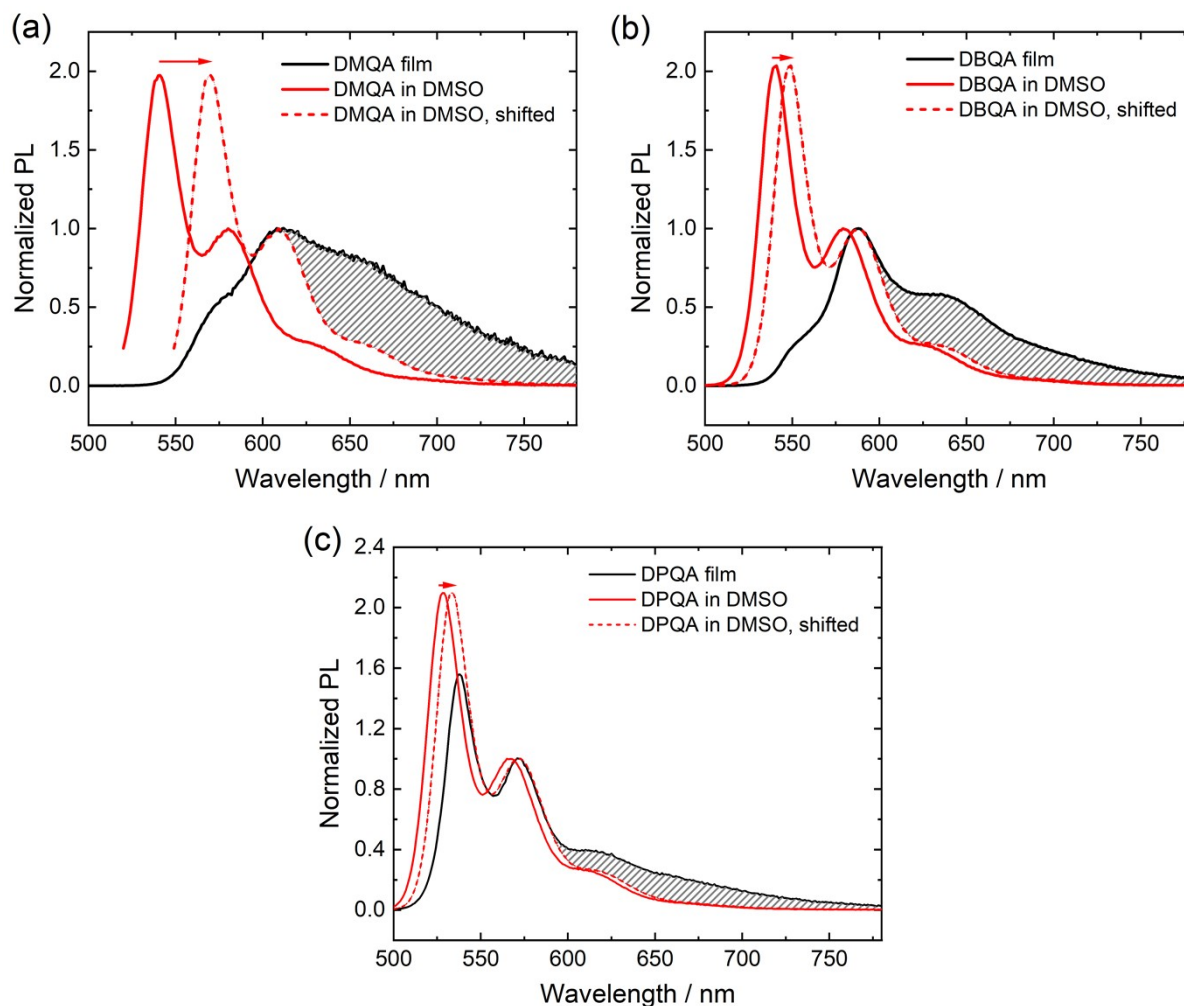


Figure S1: Normalized PL spectra measured for dilute solutions in DMSO (solid red lines) and thin films on quartz glass (solid black lines) for (a) DMQA, (b) DBQA and (c) DPQA. The spectra were normalized to the second peak in the vibronic peak progression. For comparison of the spectral shapes, the spectra measured for DMSO solutions were shifted on the wavelength scale to match the vibronic peak positions with the thin film spectra, as indicated by the red arrows. The shifted spectra are shown as dashed red lines. For qualitative comparison of the spectral shape differences in the low energy regions for the different materials, the differences are highlighted as grey hatched areas.

The absolute measured absorbance and photoluminescence spectra for the DMQA, DBQA and DPQA films are shown in **Figure S2**. The measurements were performed under equal conditions (e.g. sample placement, slit widths, excitation intensity) for each sample. The absorbance values (in a.u.) of the films at the PL excitation wavelength of $\lambda_{\text{ex}} = 470$ nm are 0.145 for DMQA, 0.199 for DBQA and 0.064 for DPQA.

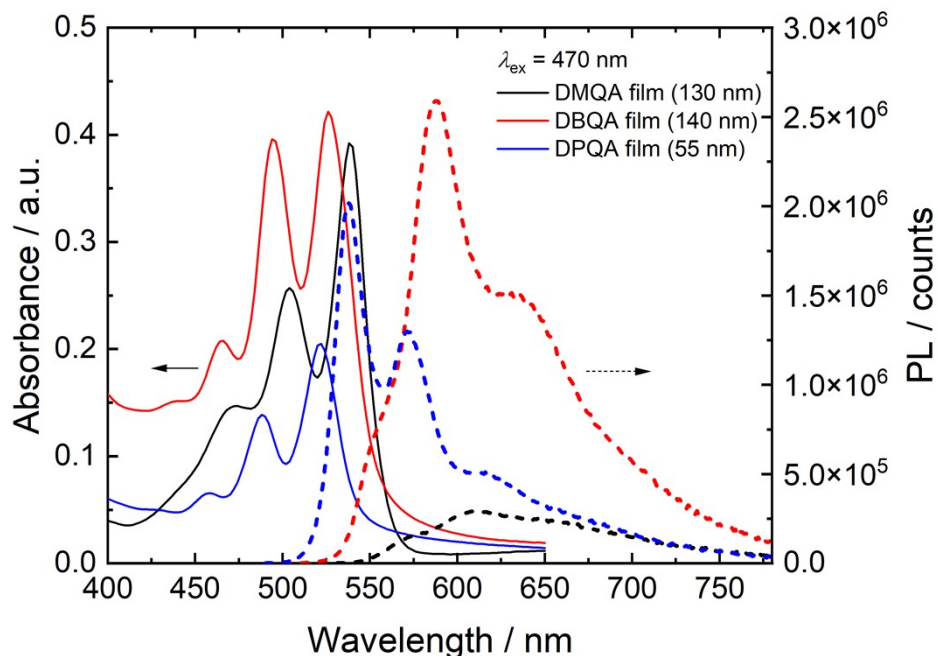


Figure S2: Absorbance (solid lines) and PL spectra (dashed lines) measured for thin films of the three *N,N'*-substituted quinacridone derivatives with film thicknesses of 130 nm (DMQA), 140 nm (DMQA) and 55 nm (DPQA).

Concentration-dependent Steady-state PL spectra

The PL spectra of solutions of DMQA and DBQA at different concentrations in DMSO are shown in **Figure S3**. The spectra are normalized to the second peak in the vibronic peak progression.

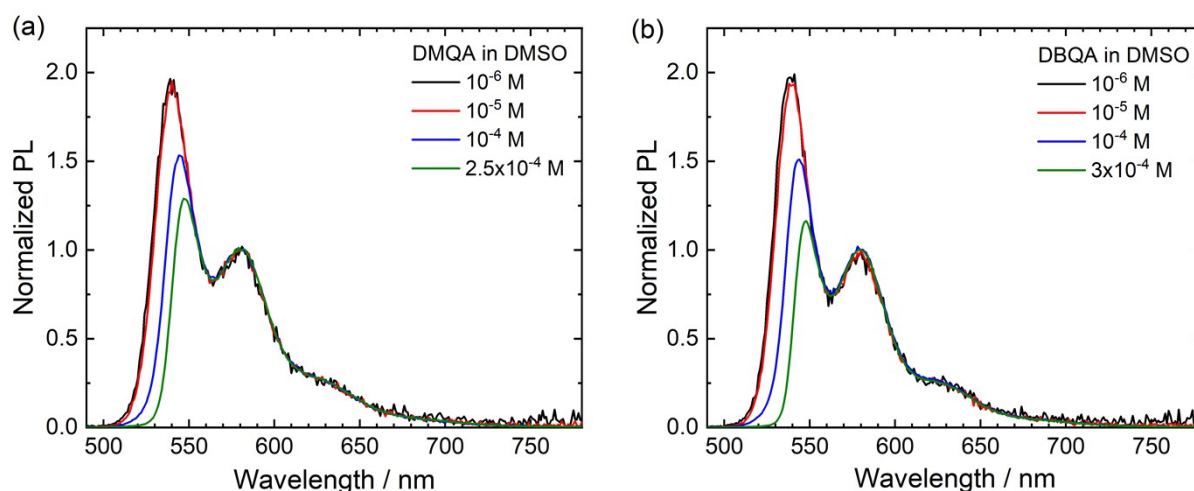


Figure S3: Normalized PL spectra of solutions of (a) DMQA and (b) DBQA in DMSO at various concentrations. The spectra were normalized to the second peak in the vibronic peak progression.

PL spectra at various concentrations were also measured for DBQA in chloroform, due to the higher solubility of the material in this solvent. The normalized PL spectra are shown in **Figure S4**.

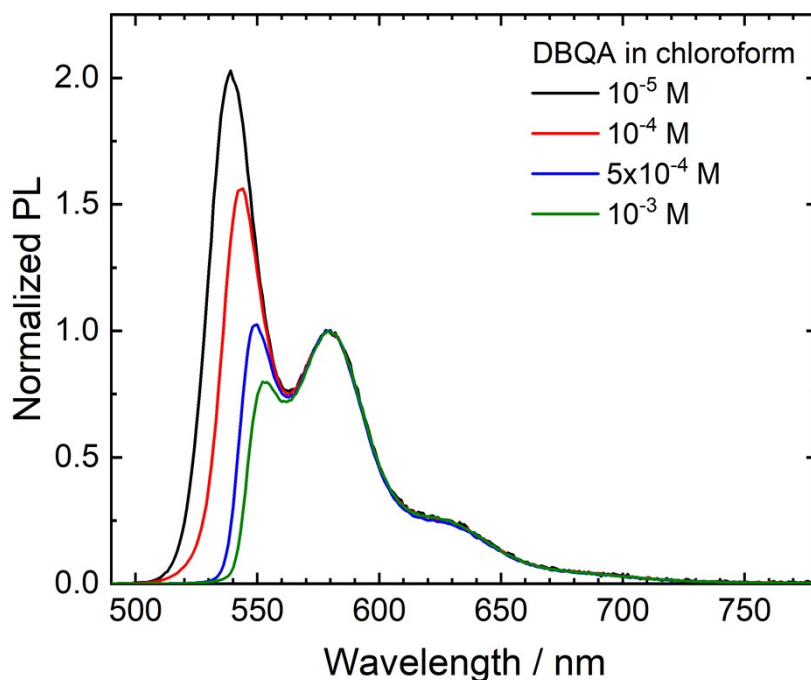


Figure S4: Normalized PL spectra of solutions of DBQA in chloroform at different concentrations. The spectra were normalized to the second peak in the vibronic peak progression.

Time-resolved Photoluminescence Fitting

The measured time-resolved PL spectra (see Figure 5) were fitted by exponential decay functions of the form:

$$y(t) = y_0 + \sum_i A_i e^{-\frac{t}{\tau_i}}$$

where y_0 is a constant, A_i is the amplitude of the decay component i , and τ_i is the decay time constant of the decay component i . For the solutions of the investigated N,N' -substituted quinacridones in DMSO, a monoexponential decay function was used for fitting. The decay curves of the thin film samples showed a more complex decay behavior and were fitted with bi- or tri-exponential functions for DMQA and DBQA, respectively, and with mono- or bi-exponential functions for DPQA. For each material, the decay curves measured at different emission wavelengths were fitted with the same set of decay time constants.

The parameters used for the fitting of the PL decay curves are summarized in **Table S1**.

Table S1: Fitting parameters for the exponential fits of the PL decay curves.

λ_{em} / nm	τ_1 / ns	τ_2 / ns	τ_3 / ns	$a_1^{(1)}$ (A_1)	$a_2^{(1)}$ (A_2)	$a_3^{(1)}$ (A_3)	y_0	R^2	$\tau_{avg}^{(2)}$ / ns
DMSO Solutions									
DMQA in DMSO									
540	18.67			1 (1.013)			0.010	0.9950	18.67
580	18.67			1 (0.969)			0.010	0.9906	18.67
625	18.67			1 (0.878)			0.010	0.9688	18.67
DBQA in DMSO									
540	18.92			1 (0.984)			0.010	0.9916	18.92
580	18.92			1 (0.940)			0.010	0.9841	18.92
625	18.92			1 (0.835)			0.015	0.9319	18.92
DPQA in DMSO									
529	16.53			1 (0.941)			0.008	0.9948	16.53
567	16.53			1 (0.969)			0.008	0.9896	16.53
610	16.53			1 (0.835)			0.020	0.9573	16.53
Thin films									
DMQA film									
570	0.24	0.59	-	0.851 (1.148)	0.149 (0.201)	-	0.0004	0.9992	0.29
615	0.24	0.59	2.07	0.679 (0.899)	0.296 (0.392)	0.025 (0.033)	0.0020	0.9991	0.39
650	0.24	0.59	2.07	0.362 (0.433)	0.526 (0.630)	0.112 (0.134)	0.0070	0.9994	0.63
700	-	0.59	2.07	-	0.770 (0.888)	0.230 (0.265)	0.0090	0.9990	0.93
DBQA film									
550	0.55	1.67	-	0.620 (0.639)	0.380 (0.391)	-	0.0013	0.9994	0.98
585	0.55	1.67	7.17	0.522 (0.577)	0.463 (0.512)	0.015 (0.017)	0.0013	0.9994	1.17
630	0.55	1.67	7.17	0.192 (0.203)	0.721 (0.763)	0.087 (0.092)	0.0015	0.9993	2.00
700	-	1.67	7.17	-	0.804 (0.888)	0.196 (0.217)	0.0087	0.9945	2.75
DPQA film									
538	0.58	1.49	-	0.880 (0.942)	0.120 (0.128)	-	0.0003	0.9992	0.69
572	0.58	1.49	-	0.847 (0.927)	0.153 (0.167)	-	0.0003	0.9995	0.72
616	0.58	1.49	-	0.296 (0.319)	0.704 (0.760)	-	0.0048	0.9983	1.22
650	-	1.49	-	-	1 (1.246)	-	0.0078	0.9975	1.49
700	-	1.49	-	-	1 (1.264)	-	0.0089	0.9953	1.49

$$a_i = \frac{A_i}{\sum_i A_i}$$

⁽¹⁾ a_i is the relative amplitude of decay component i, according to:

$$\tau_{avg} = \sum_i a_i \tau_i$$

⁽²⁾ The amplitude-weighted average PL decay time, τ_{avg} , was calculated according to:

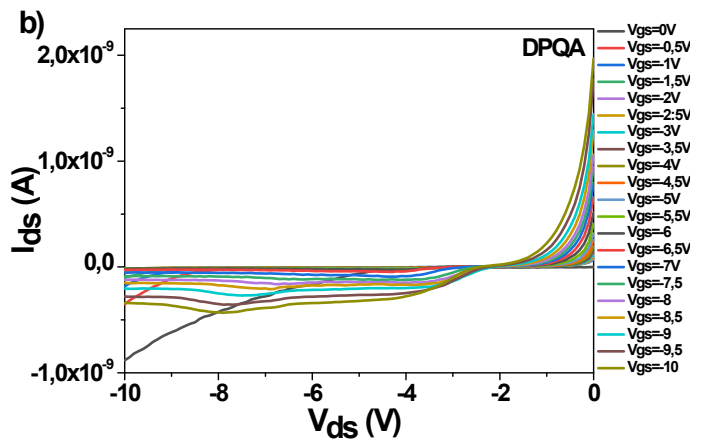
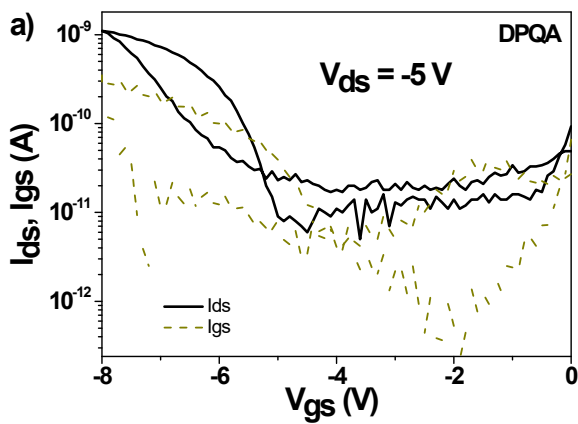


Figure S5: a) transfer and b) output characteristics of N,N'-diphenylquinacridone. Field effect mobilities: $\mu_h = 2 \times 10^{-5} \text{ cm}^2/\text{Vs}$, $\mu_e = 5 \times 10^{-6} \text{ cm}^2/\text{Vs}$. The specific capacitance of the AlOx + beeswax is $131 \text{ nF}/\text{cm}^2$.