Efficient Collection of Excitation Energy from a Linear-Shaped Weakly Interacted Perylenetetracarboxylic Diimides Array

Guiju Qi, a Lilin Jiang, b Yingyuan Zhao, a Yanqiang Yang b,* and Xiyou Li b,*

aKey Laboratory of Colloid and Interface Chemistry, Ministry of Education, Department of Chemistry, Shandong University, Jinan 250100, China; bCenter for Condensed Matter Science and Technology, Department of Physics, Harbin Institute of Technology, Harbin 150001, China.

List of Contents:
(1) Additional Spectroscopic data
   • Fluorescence spectra of compound PO-PO-PN.
   • Fluorescence spectra of compound PO-PO-PO-PN.
(2) Calculation of energy transfer parameters following the Förster theory
(3) Transient absorption spectra of PO-PN, PO-PO-PN, and PO-PO-PO-PN
(4) Decay profiles of PO-PO-PO-PN and the fitting results
Additional Spectroscopic data

**Figure S1.** Fluorescence spectra of PO-PO-PN (black line), PO (red line), PN (green line) in CH$_2$Cl$_2$, $\lambda_{ex} = 510$ nm, [PO-PO-PN] = [PO] = [PN] = $5 \times 10^{-6}$ mol L$^{-1}$. The inset indicates the expanded emission spectra of PO-PO-PN and PN.

**Figure S2.** Fluorescence spectra of PO-PO-PO-PN (black line), PO (red line), PN (green line) in CH$_2$Cl$_2$, $\lambda_{ex} = 510$ nm, [PO-PO-PO-PN] = [PO] = [PN] = $5 \times 10^{-6}$ mol L$^{-1}$. The inset indicates the expanded emission spectra of PO-PO-PO-PN and PN clearly.
Calculation of energy transfer parameters following the Föster model

According to the Förster theory, the rate for energy transfer $k_{\text{EnT}}$ for a donor (D) and acceptor (A) molecule separated by a distance $R$ is given by:[1]

$$k_{\text{EnT}}(r) = \frac{\phi_D \lambda^2}{\tau_D} \left( \frac{9000(\ln 10)}{128\pi^5 N \eta^4} \right) \int_0^\infty F_D(\lambda) \varepsilon_A(\lambda) \lambda^4 d\lambda$$

(S-1)

where $\phi_D$ is the quantum yield of fluorescence of the donor, $\kappa^2$ is a factor describing the orientation of the transition dipoles with respect to each other, $\eta$ is the refractive index of the solvent, $\tau_D$ is the fluorescence lifetime of the donor, $F_D(\lambda)$ is the normalized fluorescence intensity of the donor and $\varepsilon_A(\lambda)$ is the extinction coefficient of the acceptor. The distance at which Förster energy transfer is considered to be 50% efficient is known as the Förster radius, $R_0$, and can be calculated using eq. S-2.

$$R_0^6 = \left( \frac{9000(\ln 10) \phi_D \kappa^2}{128\pi^5 N \eta^4} \right) \int_0^\infty F_D(\lambda) \varepsilon_A(\lambda) \lambda^4 d\lambda$$

(S-2)

Using $R_0$ from eq S-2, the Förster energy transfer efficiencies of the compounds can be estimated from the on or to acceptor distance, $r$, and

$$\phi_{\text{EnT}} = \frac{R_0^6}{R_0^6 + r^6}$$

(S-3)

Using eqs S1-S3, the FRET rates and efficiencies were estimated.[2] where $n_{\text{DCM}} = 1.424$. The orientation factor used was $\kappa^2 = 4$. The donor acceptor distances were calculated using quantum chemical calculations and the computational results are found in Table 4 of the main text. The fluorescence spectrum was obtained from PO and the absorption spectrum was obtained from PN. The PO fluorescence quantum yield is 0.80. The extinction coefficient of PN and PO is 51400 $\text{M}^{-1}\text{cm}^{-1}$ at 700 nm and 53600 $\text{M}^{-1}\text{cm}^{-1}$ at 573 nm.
REFERENCES


(3) Transient absorption spectra of PO-PN, PO-PO-PN, and PO-PO-PO-PN

Figure S3. Transient absorption spectra of PO-PN.

Figure S4. Transient absorption spectra of PO-PO-PN.
**Figure S5.** Transient absorption spectra of PO-PO-PO-PN
The decay traces and fitting results of PO-PO-PO-PN

**Figure S6.** The decay traces of the ground state bleaching of PO-PO-PO-PN at 600 nm (up) and 710 nm (down) and the fitting results.