**Supporting Information**

# The Influence of Intermolecular Orientation on the Photoinduced Charge Transfer Kinetics in Self-assembled Aggregates of Donor-Acceptor Arrays

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Table S1: Evolution of the total energy of the dimer (in kcal/mol) as a function of the average distance between the perylene bisimide nitrogen atoms in the two interacting molecules for **1**, **2** and **3**, as calculated at the UFF level.

| **1** | | **2** | | **3** | |
|---|---|---|---|---|---|
| *d*(N1-N2) | Energy | *d*(N1-N2) | Energy | *d*(N1-N2) | Energy |
| 4.48 | 568.44 | 3.83 | 685.06 | 5.14 | 621.87 |
| 5.58 | 568.93 | 4.40 | 669.82 | 5.24 | 609.73 |
| 5.51 | 561.86 | 4.57 | 673.71 | 6.06 | 621.48 |
| 5.51 | 554.72 | 4.54 | 676.40 | 11.73 | 628.68 |
| 11.53 | 567.72 | 9.60 | 696.68 | 11.18 | 617.50 |
| 8.99 | 584.50 | 9.78 | 697.31 | 11.26 | 616.13 |
| 12.26 | 568.15 | 10.01 | 696.46 | 11.22 | 615.98 |
| 12.33 | 568.07 | 11.59 | 696.91 | 11.53 | 619.53 |
| 12.45 | 568.81 | 11.46 | 695.10 | 11.58 | 619.97 |
| 11.31 | 563.72 | 11.37 | 696.88 | 11.50 | 618.29 |
| 11.30 | 563.57 | 11.16 | 699.41 | 11.48 | 618.06 |
| 18.39 | 578.10 | 15.54 | 708.74 | 17.90 | 631.09 |
| 18.37 | 579.33 | 16.34 | 714.32 | 18.34 | 627.56 |

The circular dichroism spectra are recorded for compounds **1**, **2**, and **3** in MCH (Figure S1). The detected maximum signal in the circular dichroism spectrum is –2 mdeg at 462 nm for compound **1**. For compound **2**, a broad signal is observed with $\lambda_{min}$ = 447 nm (-7 mdeg) and $\lambda_{max}$ = 594 nm (+5 mdeg). For compound **3**, a bisignated signal is detected with $\lambda_{min}$ = 472 nm (-2 mdeg) and $\lambda_{max}$ = 416 nm (+2 mdeg). All spectra are recorded at a concentration of $5 \times 10^{-5}$M in MCH in a 10 mm cell.

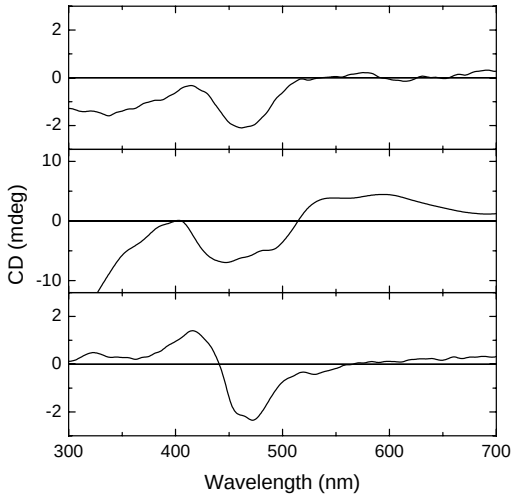


Figure S1: Circular dichroism spectra of $5 \times 10^{-5}$M solutions of **1** (top), **2** (middle) and **3** (bottom) in MCH recorded at 20 °C in an absorption cell with a 10 mm path length.