Supporting Information

Ultrafast Photoinduced Intramolecular Charge Separation and Recombination Processes in the Oligothiophene-Substituted Benzene Dyads with a Amide Spacer

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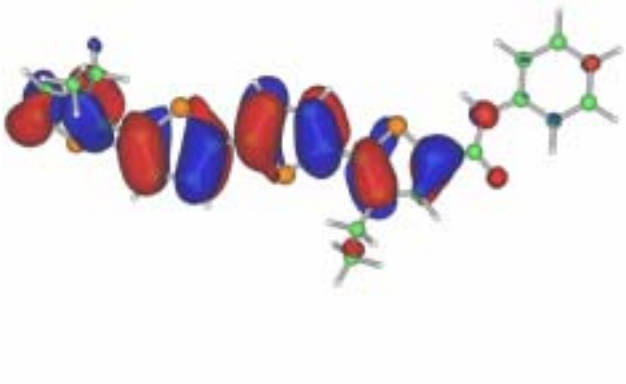
(A) HOMO



(B) LUMO

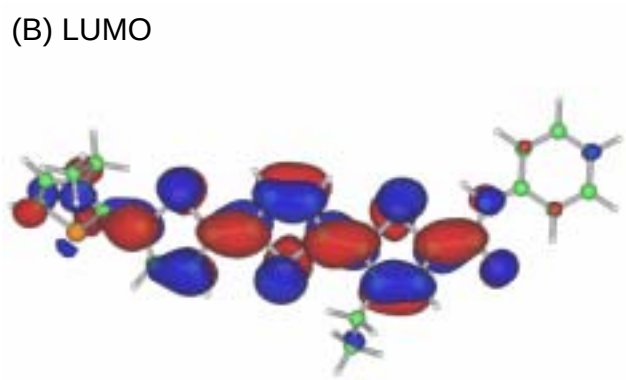


Figure S1. Optimized structures and electron densities of the HOMO (A) and LUMO (B) of **1** calculated at the B3LYP/6-31G(d) level, using ethyl groups instead of hexyl groups.

Table S1: Photophysical properties of 1, 2, and 3.

Compound	Solvent	λ_{abs} / nm	λ_{fl} / nm	ϕ_{fl} [a]	τ_{fl} / ps	ϕ_T [b]	τ_T / μs
1	Tol	397	483	0.15	460	0.35	25
	ANS	402	492	0.14	460	0.33	31
	THF	395	481	0.16	470	0.34	23
	PhCN	403	518	0.12	480	0.35	31
	MeCN	394	509	0.12	470	0.32	19
2	Tol	391	494	0.13	440	0.34	27
	ANS	395	507	0.12	450	0.37	38
	THF	387	496	0.12	440	0.31	36
	PhCN	397	515	0.11	440	0.42	42
	MeCN	385	513	0.11	440	0.34	22
3	Tol	395	502	0.13	460	0.35	28
	ANS	398	515	0.12	430	0.32	40
	THF	393	507	0.12	440	0.36	37
	PhCN	400	523	0.10	460	0.35	40
	MeCN	388	524	0.09	460	0.36	24

[a] Using tetrathiophene as a reference. [b] Estimated by assuming the extinction coefficients at peak of the dyads in the triplet excited states are same with that of **4** in benzene and using benzophenone as a reference.