

Supplement Files

Self-Assembly Behavior, Aggregation Structure, and the Charge Carrier Transport Properties of S-Heterocyclic Annulated Perylene Diimide Derivatives

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1. DFT-optimized molecular conformations and the calculated intermolecular distance of linear SPDI and dendronized SPDI

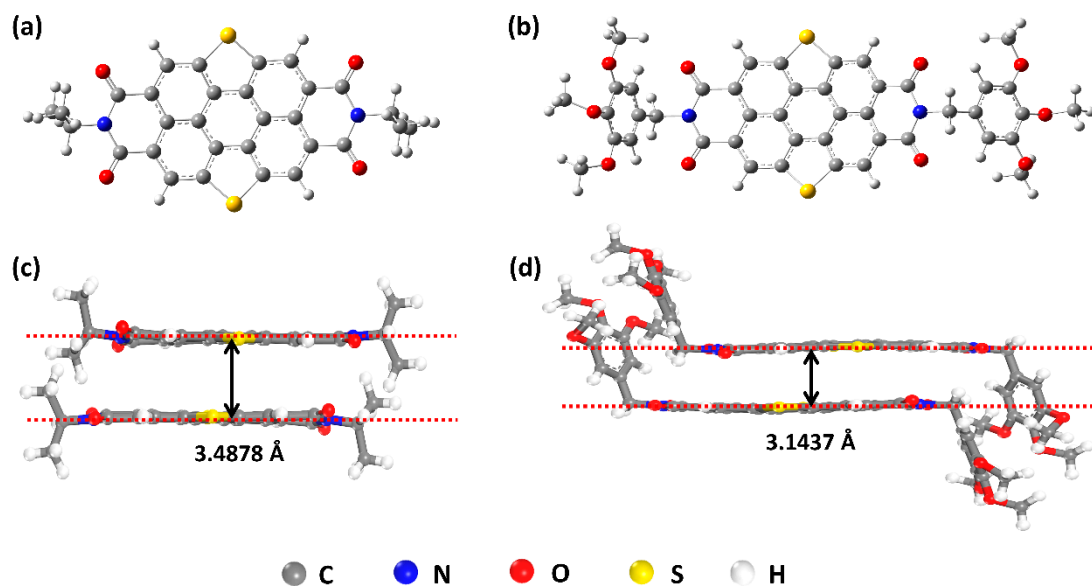


Figure S1. DFT-optimized molecular conformations of (a) linear SPDI and (b) dendronized SPDI, and the calculated intermolecular distance of (c) linear SPDI (3.4878 Å) and (d) dendronized SPDI (3.1437 Å).

2. The crystallographic parameters of linear SPDI

Table S1. Crystallographic parameters of linear SPDI

<i>(hkl)</i>	2 θ (deg)		<i>d</i> -spacing (nm)		Intensity
	expt ^a	calcd ^b	expt ^a	calcd ^b	expt ^c
100	2.80	2.80	3.16	3.16	w
010	3.00	3.00	2.95	2.95	vs
-110	3.75	3.75	2.36	2.36	vw
020	6.00	6.00	1.47	1.47	s
-220	7.50	7.50	1.18	1.18	vw
030	9.00	9.01	0.98	0.98	s
-330	11.00	11.27	0.80	0.79	vw
060	18.00	18.07	0.49	0.49	w
540	20.00	19.99	0.44	0.44	m
630	20.70	20.43	0.43	0.43	w
640	22.00	22.34	0.40	0.40	w
650	23.60	24.48	0.38	0.36	m
660	26.00	26.81	0.34	0.33	m
011	8.60	8.92	1.03	0.99	m
021	9.90	10.33	0.89	0.86	m
-321	12.70	12.69	0.70	0.70	m
-331	14.00	14.07	0.63	0.63	m
331	15.80	15.76	0.56	0.56	w
-341	16.50	15.91	0.54	0.56	w
541	21.00	21.71	0.42	0.41	w
022	17.00	17.90	0.52	0.50	w
032	18.80	19.13	0.47	0.46	vs
033	25.60	26.98	0.35	0.33	w

3. The direct image of self-assembly of linear SPDI

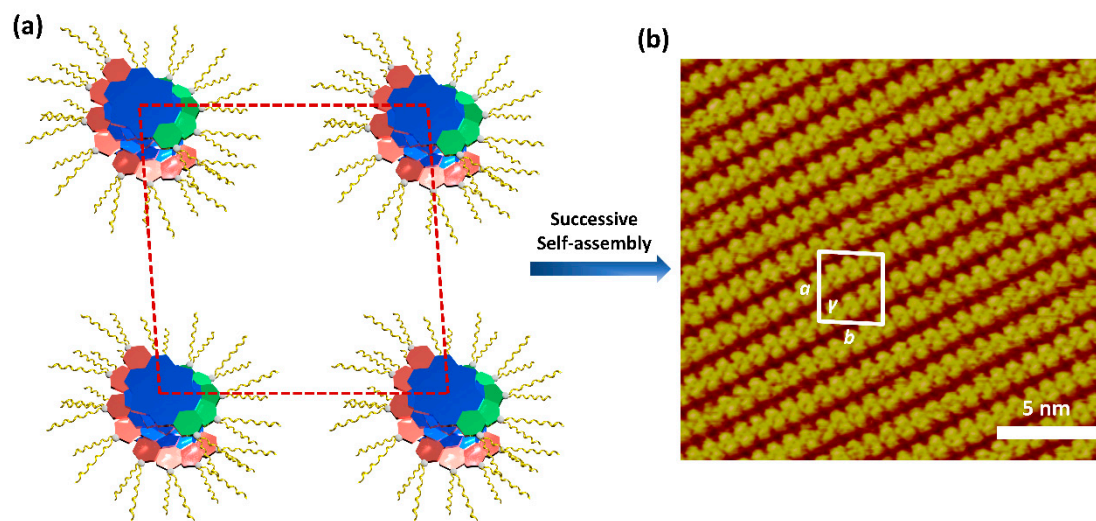


Figure S2. (a) Model of the helical column in the monoclinic lattice of linear SPDI; (b) high-resolution STM image of linear SPDI.

4. The ^1H NMR spectrum of compound 2 recorded in CDCl_3

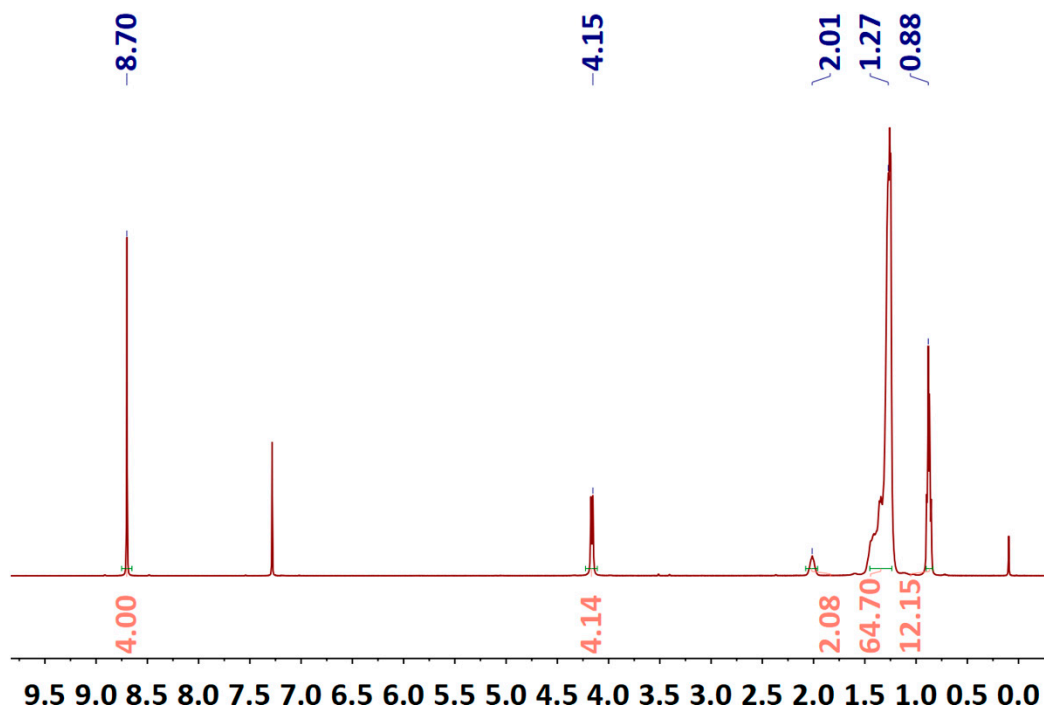


Figure S3. ^1H NMR spectrum of compound 2.

5. The ^1H NMR spectrum of linear SPDI recorded in CDCl_3 .

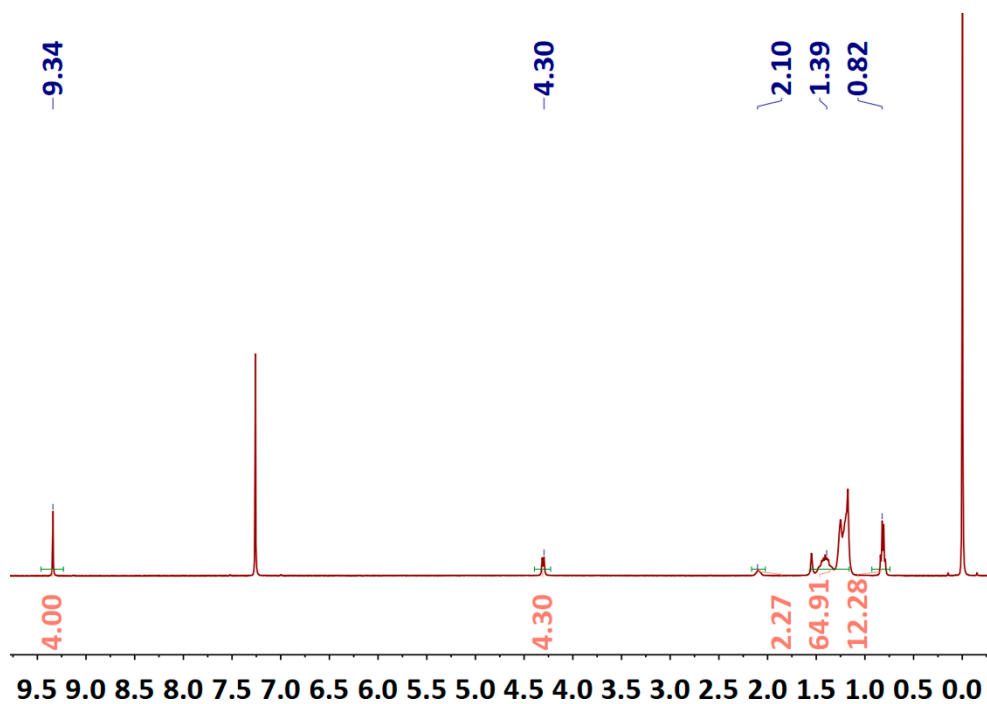


Figure S4. ^1H NMR spectrum of linear SPDI.

6. The ^1H NMR spectrum of dendronized SPDI recorded in CDCl_3 .

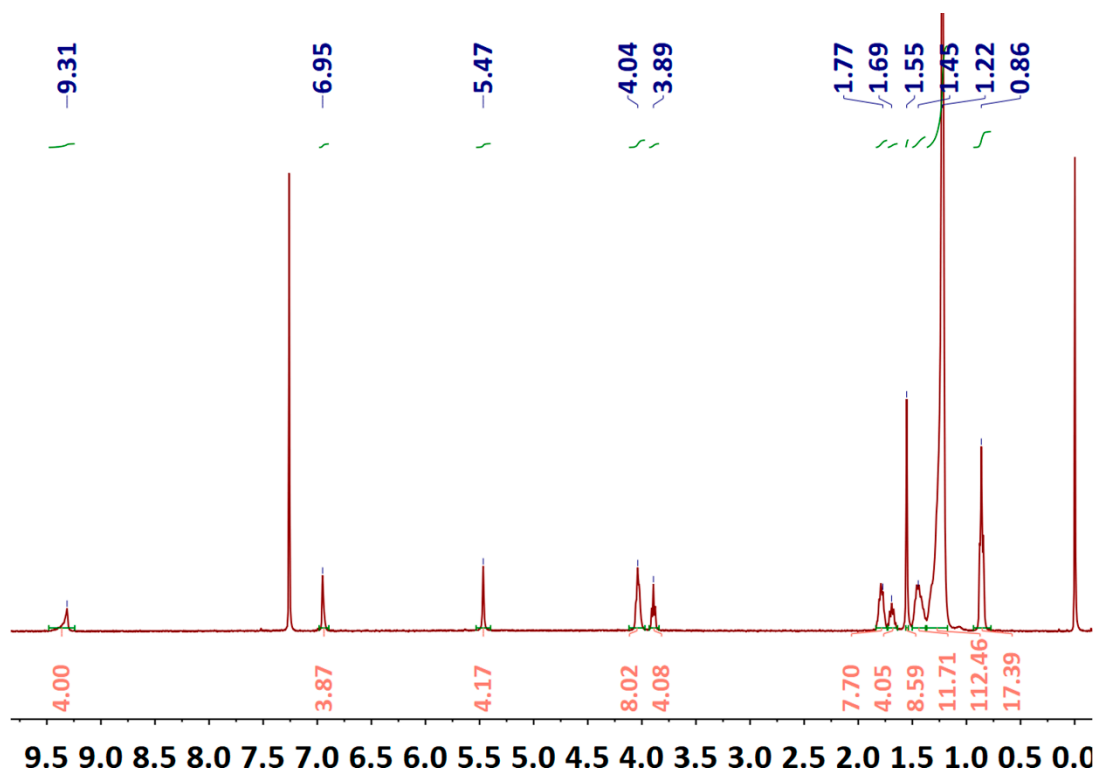


Figure S5. ^1H NMR spectrum of dendronized SPDI.