Supporting Information

Dithiazole-fused Naphthalene Diimides toward New n-type Semiconductors

Xin Chen, Yunlong Guo, Luxi Tan, Ge Yang, Yonghai Li, Guanxin Zhang,* Zitong Liu, Wei Xu and Deqing Zhang*

Beijing National Laboratory for Molecular Sciences, Organic Solids Laboratory, Institute of Chemistry, Chinese Academy of Sciences, Beijing 100190, China.

E-mail: dqzhang@iccas.ac.cn

Contents:

1. ^{1}H NMR and ^{13}C NMR spectra of 1 and 2 as well as those of 1 + 1' and 2 + 2'

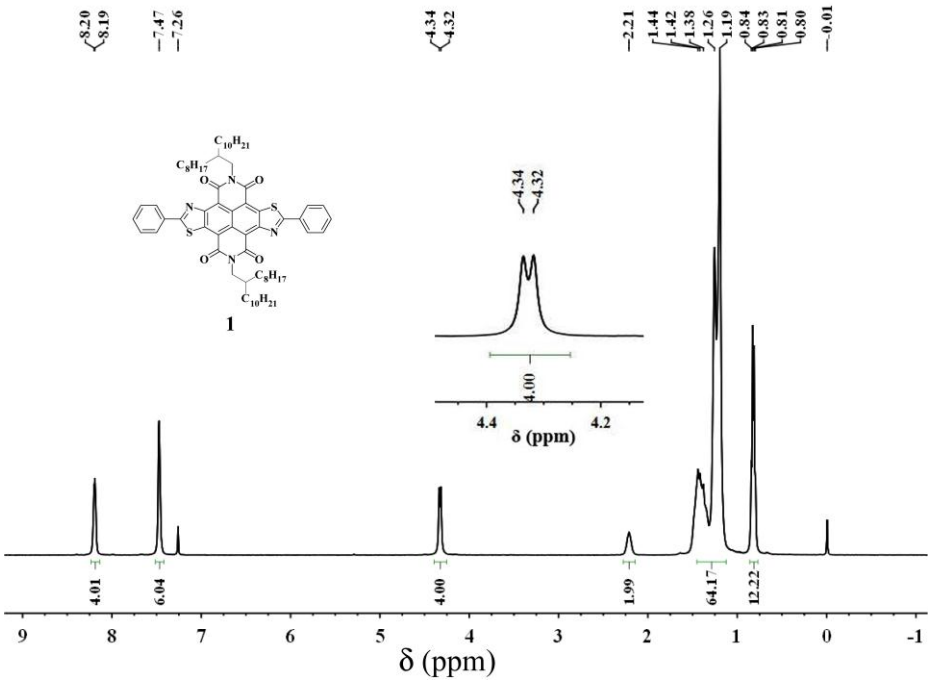

Fig. S1 ^{1}H NMR spectra of **1**

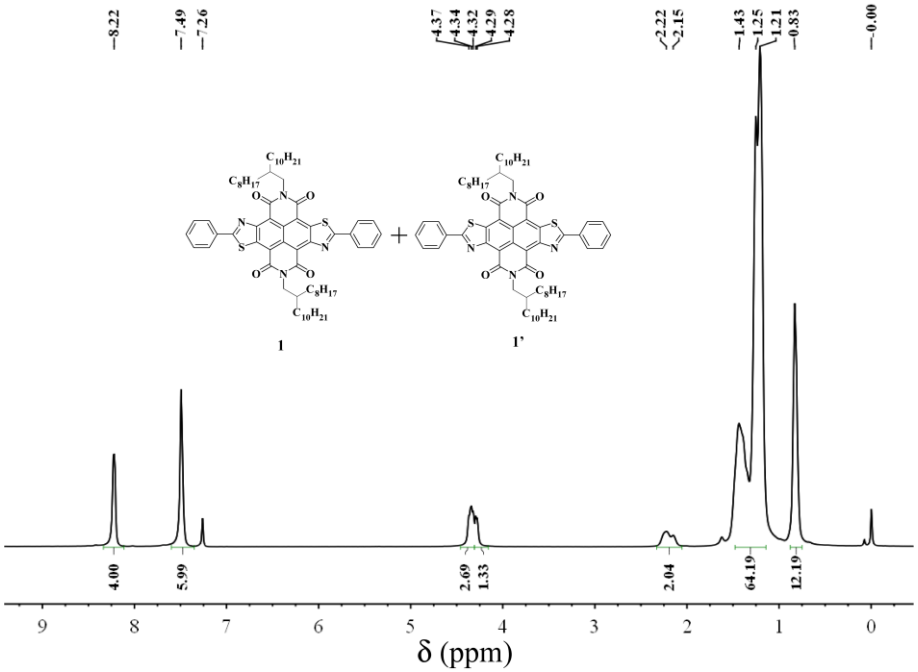

Fig. S2 ^{1}H NMR spectra of **1** + **1'**

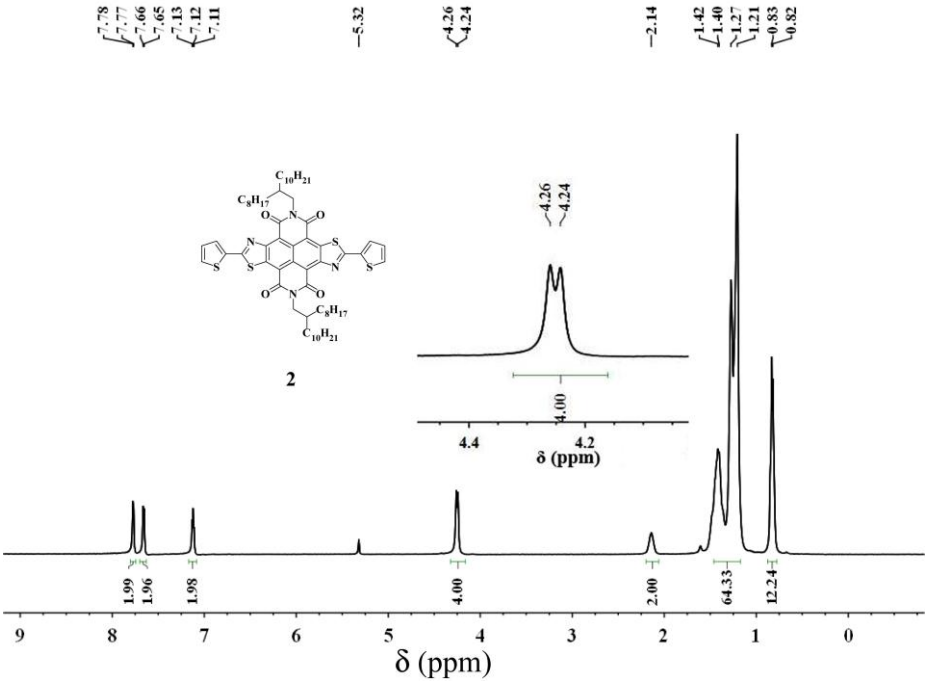

Fig. S3 ^{1}H NMR spectra of **2**

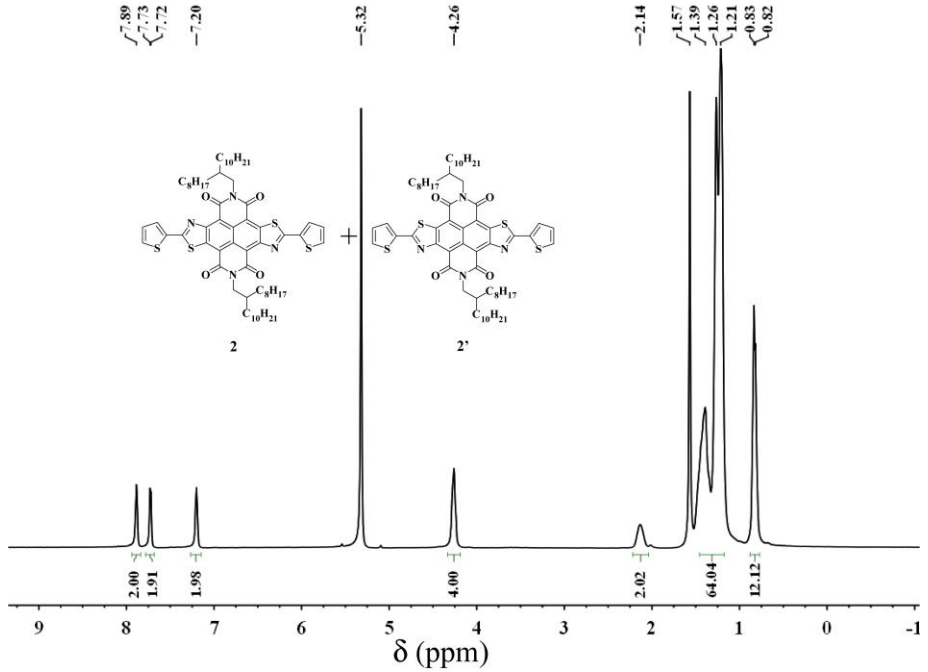

Fig. S4 ^{1}H NMR spectra of **2** + **2'**

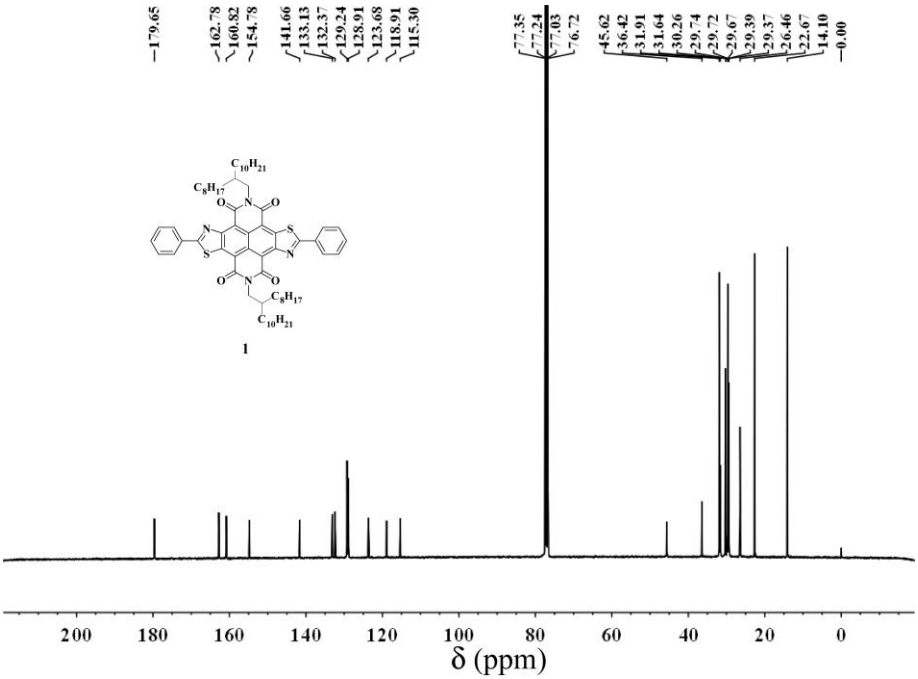

Fig. S5 ^{13}C NMR spectra of **1**

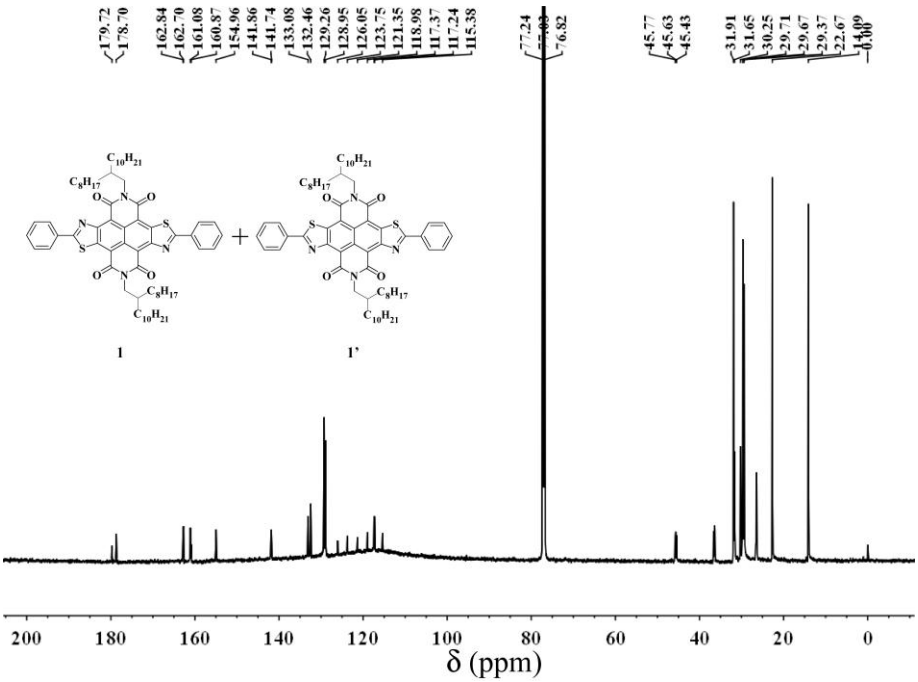

Fig. S6 ^{13}C NMR spectra of **1** + **1'**

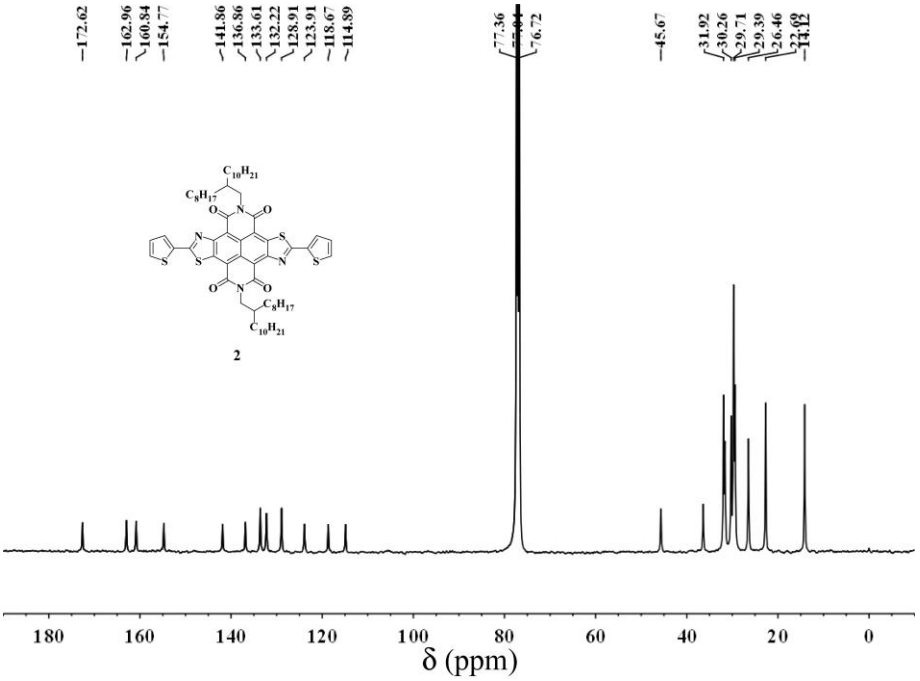

Fig. S7 ^{13}C NMR spectra of **2**

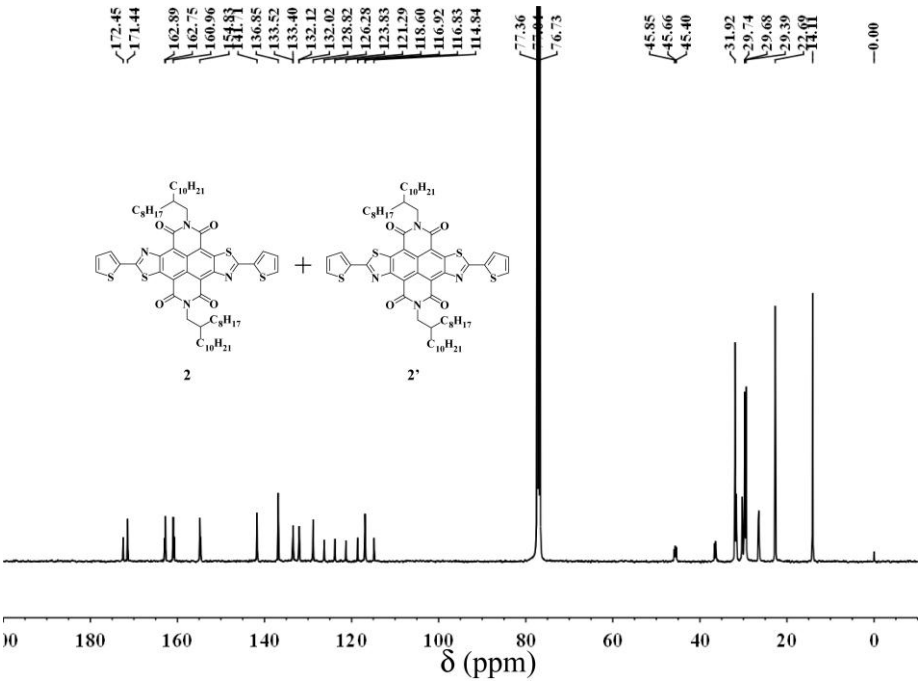

Fig. S8 ^{13}C NMR spectra of **2** + **2'**

2. TGA-DTA analysis

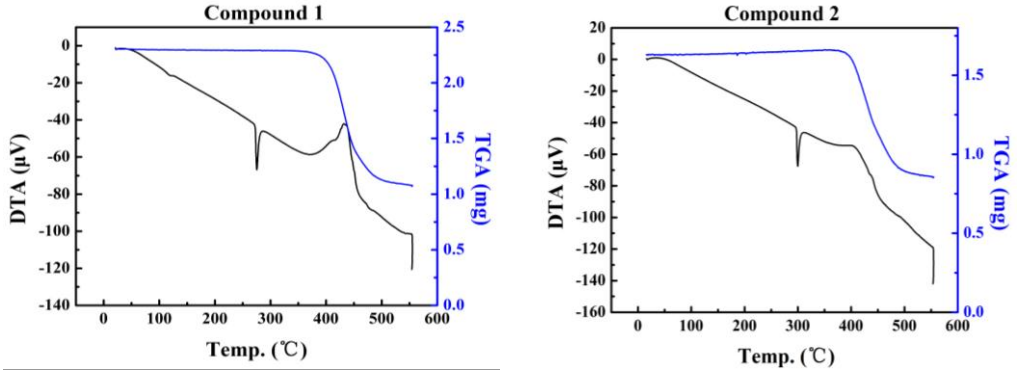

Fig. S9 TGA-DTA curves of **1** and **2** from 25 °C to 550 °C with heating rate of 10 °C/min. under nitrogen atmosphere.

3. UV-Vis absorption spectra of 2

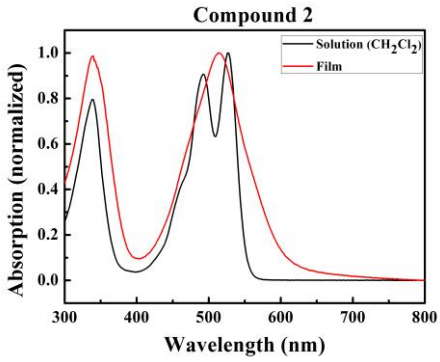

Fig. S10 Normalized absorption spectra of solutions in CH_2Cl_2 and thin films of **2** .

4. DFT calculation data

Calculation method: B3LYP/6-31G (d, p) with Gaussian 09

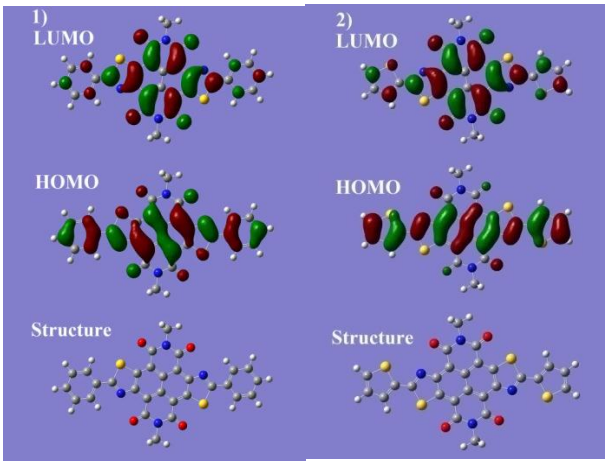

Fig. S11 LUMO/HOMO orbitals and structures of compounds **1** and **2** obtained with DFT calculations; the long N-alkyl chains were replaced by N-methyl groups in the calculations.

Calculation data for compound 1

		Coordinates		
		X	Y	Z
1	C	-2.509000	-0.435293	-0.000005
2	C	-2.310541	0.987890	-0.000028
3	C	-1.047874	1.555344	-0.000084
4	C	0.094268	0.712427	-0.000025
5	C	-0.090615	-0.712951	-0.000001
6	C	-1.392775	-1.284989	-0.000008
7	C	1.395650	1.286762	0.000016
8	C	2.511522	0.435557	0.000021
9	C	2.312897	-0.988345	0.000029
10	C	1.050532	-1.557716	0.000040
11	C	0.916562	-3.028514	0.000084
12	N	-0.376091	-3.535849	0.000043
13	C	-1.557476	-2.764052	-0.000047
14	C	-0.908437	3.023387	-0.000165
15	N	0.379058	3.536437	-0.000502
16	C	1.566656	2.767455	0.000171
17	O	-2.631826	-3.339743	-0.000158
18	O	2.649501	3.325916	0.000766
19	C	-0.562582	-4.991825	0.000048
20	C	0.494752	4.999874	-0.000616
21	O	1.902520	-3.762005	0.000143
22	O	-1.884258	3.770524	-0.000023
23	N	3.827014	0.826368	-0.000024
24	C	4.635830	-0.192765	-0.000014
25	S	3.853994	-1.804921	0.000060
26	N	-3.824230	-0.827026	0.000034

27	C	-4.633167	0.192088	0.000030
28	S	-3.851170	1.804997	-0.000028
29	C	6.093287	-0.045663	-0.000028
30	C	6.954034	-1.156091	-0.000399
31	C	8.334237	-0.974253	-0.000382
32	C	8.870657	0.315112	0.000005
33	C	8.020541	1.425052	0.000365
34	C	6.641175	1.251286	0.000349
35	C	-6.090624	0.045191	0.000052
36	C	-6.951259	1.155686	0.000331
37	C	-8.331478	0.973959	0.000334
38	C	-8.868004	-0.315359	0.000058
39	C	-8.017981	-1.425367	-0.000214
40	C	-6.638593	-1.251733	-0.000217
41	H	0.421494	-5.452911	0.000296
42	H	-1.129089	-5.290269	0.884159
43	H	-1.128653	-5.290343	-0.884321
44	H	1.552402	5.248000	-0.004936
45	H	-0.001654	5.408023	-0.883306
46	H	0.006117	5.407997	0.886495
47	H	6.548892	-2.163815	-0.000729
48	H	8.991120	-1.838512	-0.000674
49	H	9.947636	0.454476	0.000023
50	H	8.435965	2.428171	0.000664
51	H	5.964148	2.098370	0.000627
52	H	-6.546020	2.163373	0.000565
53	H	-8.988282	1.838279	0.000555
54	H	-9.944995	-0.454634	0.000059
55	H	-8.433470	-2.428458	-0.000428

56	H	-5.961686	-2.098923	-0.000420

Total energy: -2469.26490606 Hartrees

Calculation data for compound 2:

		Coordinates		
		X	Y	Z
1	C	2.525894	-0.349330	0.000000
2	C	2.275471	1.066677	-0.000011
3	C	0.994614	1.591404	-0.000001
4	C	-0.117643	0.708549	0.000075
5	C	0.117642	-0.708550	0.000055
6	C	1.437964	-1.236191	-0.000010
7	C	-1.437965	1.236192	0.000132
8	C	-2.525895	0.349331	0.000104
9	C	-2.275472	-1.066677	0.000156
10	C	-0.994615	-1.591407	0.000122
11	C	-0.812272	-3.056217	0.000180
12	N	0.495407	-3.520106	-0.000035
13	C	1.651271	-2.708542	-0.000139
14	C	0.812268	3.056213	-0.000096
15	N	-0.495411	3.520105	-0.000115
16	C	-1.651276	2.708544	0.000290
17	O	2.743735	-3.247756	-0.000431
18	O	-2.743742	3.247752	0.000674
19	C	0.730781	-4.968976	-0.000186
20	C	-0.730760	4.968977	-0.000147
21	O	-1.775211	-3.820859	0.000318
22	O	1.775207	3.820857	-0.000234
23	N	-3.854242	0.694439	0.000032
24	C	-4.620745	-0.360432	0.000063

25	S	-3.784421	-1.944166	0.000205
26	C	-6.058875	-0.282965	-0.000001
27	N	3.854242	-0.694439	0.000048
28	C	4.620745	0.360432	0.000063
29	S	3.784420	1.944166	-0.000115
30	C	6.058875	0.282964	0.000095
31	C	6.987826	1.306873	0.000572
32	C	8.325923	0.840176	0.000498
33	C	8.401212	-0.531299	-0.000034
34	S	6.845995	-1.281259	-0.000467
35	C	-6.987828	-1.306872	0.000451
36	C	-8.325924	-0.840174	0.000254
37	C	-8.401211	0.531301	-0.000326
38	S	-6.845995	1.281261	-0.000652
39	H	-0.237340	-5.462731	-0.001659
40	H	1.308133	-5.247874	-0.883651
41	H	1.305609	-5.248636	0.884710
42	H	0.237368	5.462724	0.000170
43	H	-1.307123	5.248234	0.883854
44	H	-1.306539	5.248310	-0.884521
45	H	6.714713	2.356206	0.000989
46	H	9.193524	1.488946	0.000838
47	H	9.292390	-1.144240	-0.000217
48	H	-6.714715	-2.356206	0.000924
49	H	-9.193526	-1.488943	0.000543
50	H	-9.292390	1.144241	-0.000599

Total energy: -3110.77005352 Hartrees

5. XRD patterns and AFM images of thin films of 2

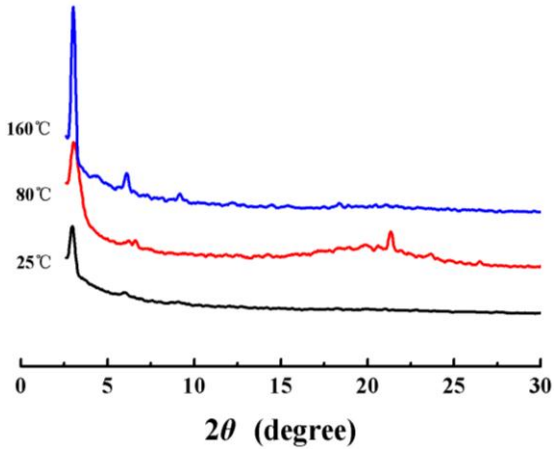

Fig. S12 XRD patterns of thin films of **2** after annealing at 25 °C, 80 °C and 160 °C, respectively.

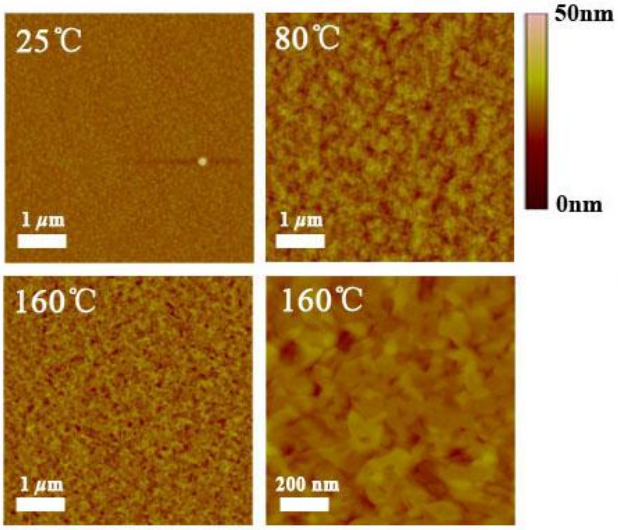

Fig. S13 AFM images of thin films of **2** after annealing at 25 °C, 80 °C and 160 °C, respectively.