One or Semi-Two Dimensional Organic Nanocrystals Induced by Directional Supramolecualr Interactions

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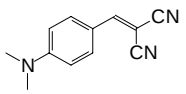
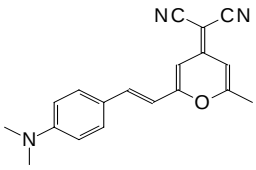
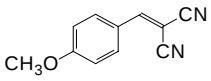
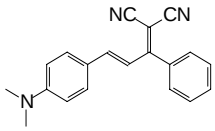
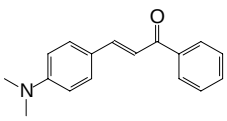
Supporting information

Part S1 Experimental section

Sample	Molecular Structure	Calculated Dipole Moment (debye)
1		11.05
2		14.79
3		8.98
4		12.11
5		6.28

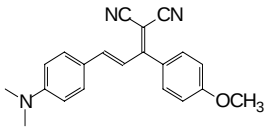
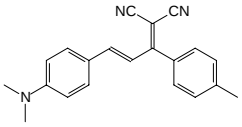
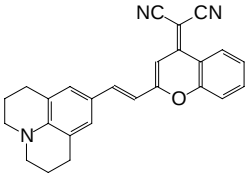
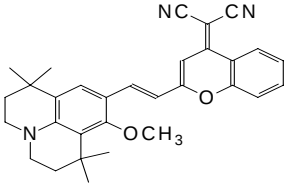
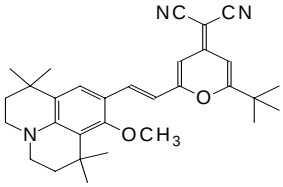
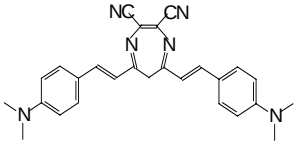
6		11.38
7		12.20
8		13.42
9		13.13
10		14.09
11		20.54

Table 1 ICT molecular structures and the corresponding calculated dipole moments

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Part S2

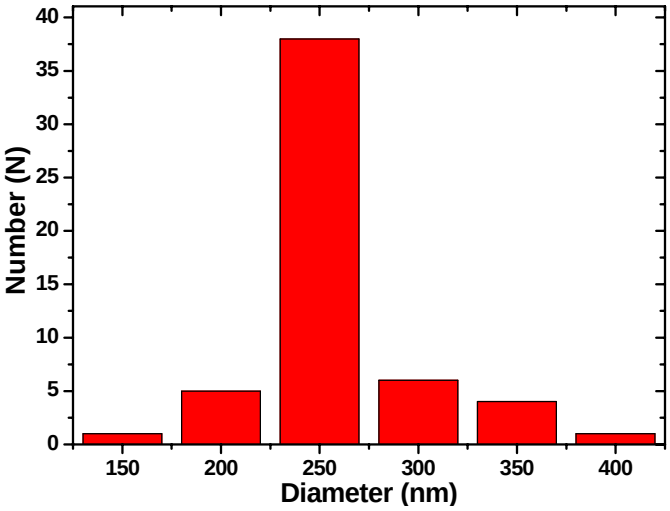


Figure S2 Statistical analysis on nanowires formed by compound 2 in the width distributions.

Part S3

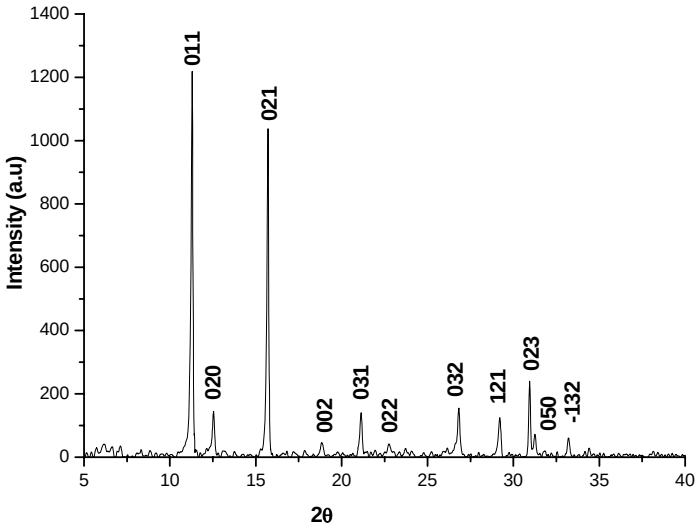


Figure S3-1 is the x-ray diffraction pattern of the nanowires of compound 1. The peaks are well indexed with program Powder-X. Indexing results of the powder diffraction pattern are shown below.

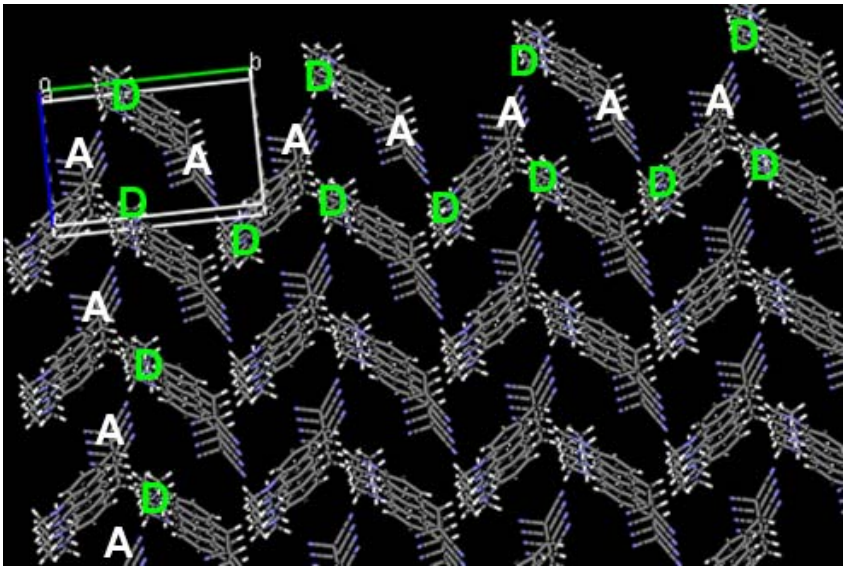
Sample Name compound 1

Crystal system: Monoclinic Lattice Type: P
Lattice Parameter: a= 3.92 b= 14.09 c= 9.62
Lattice Parameter: Alpha= 90 Beta= 99.9 Gama=90
Radiation: Cu WaveLength: 1.540598
2Theta Start= 3.01 2Theta End= 45

H	K	L	d	2Theta	SinT	SinT^2
0	1	0	14.09000	6.268	0.054670	0.002989
0	0	1	9.47675	9.325	0.081283	0.006607
0	1	1	7.86358	11.243	0.097958	0.009596
0	2	0	7.04500	12.555	0.109340	0.011955
0	2	1	5.65387	15.661	0.136243	0.018562
0	0	2	4.73838	18.712	0.162566	0.026428
0	3	0	4.69667	18.879	0.164010	0.026899
0	1	2	4.49121	19.752	0.171512	0.029417
0	3	1	4.20821	21.095	0.183047	0.033506
0	2	2	3.93179	22.596	0.195916	0.038383
-1	0	0	3.86163	23.013	0.199475	0.039790

1	0	0	3.86163	23.013	0.199475	0.039790
-1	0	1	3.81252	23.313	0.202044	0.040822
-1	1	0	3.72429	23.873	0.206831	0.042779
1	1	0	3.72429	23.873	0.206831	0.042779
-1	1	1	3.68018	24.164	0.209310	0.043811
0	4	0	3.52250	25.263	0.218680	0.047821
-1	2	0	3.38628	26.297	0.227476	0.051746
1	2	0	3.38628	26.297	0.227476	0.051746
1	0	1	3.37888	26.356	0.227975	0.051973
-1	2	1	3.35302	26.563	0.229733	0.052777
0	3	2	3.33569	26.703	0.230926	0.053327
0	4	1	3.30179	26.983	0.233297	0.054428
1	1	1	3.28572	27.117	0.234438	0.054961
-1	0	2	3.28255	27.144	0.234665	0.055067
-1	1	2	3.19694	27.885	0.240949	0.058056
0	0	3	3.15892	28.228	0.243849	0.059462
0	1	3	3.08240	28.943	0.249902	0.062451
1	2	1	3.04659	29.291	0.252839	0.063928
-1	3	0	2.98284	29.932	0.258243	0.066690
1	3	0	2.98284	29.932	0.258243	0.066690
-1	2	2	2.97542	30.008	0.258887	0.067023
-1	3	1	2.96004	30.168	0.260233	0.067721
0	2	3	2.88242	31.000	0.267241	0.071418
0	4	2	2.82693	31.624	0.272486	0.074249
0	5	0	2.81800	31.727	0.273350	0.074720
1	0	2	2.76934	32.300	0.278152	0.077369
1	3	1	2.74283	32.621	0.280841	0.078872
1	1	2	2.71735	32.935	0.283474	0.080357
0	5	1	2.70111	33.139	0.285179	0.081327
-1	3	2	2.69055	33.273	0.286298	0.081967
-1	0	3	2.68140	33.390	0.287275	0.082527
-1	1	3	2.63413	34.007	0.292431	0.085516
0	3	3	2.62119	34.180	0.293873	0.086362
-1	4	0	2.60243	34.434	0.295992	0.087611
1	4	0	2.60243	34.434	0.295992	0.087611
-1	4	1	2.58725	34.643	0.297729	0.088643
1	2	2	2.57736	34.780	0.298871	0.089324
-1	2	3	2.50602	35.803	0.307379	0.094482
1	4	1	2.43842	36.830	0.315901	0.099793
0	5	2	2.42204	37.089	0.318037	0.101148
-1	4	2	2.40147	37.418	0.320762	0.102888

1	3	2	2.38553	37.677	0.322905	0.104268
0	0	4	2.36919	37.947	0.325132	0.105711
0	4	3	2.35176	38.239	0.327541	0.107283
0	6	0	2.34833	38.297	0.328019	0.107597
0	1	4	2.33639	38.501	0.329696	0.108700
-1	3	3	2.32862	38.634	0.330796	0.109426
0	6	1	2.27939	39.503	0.337940	0.114204
-1	5	0	2.27634	39.558	0.338394	0.114510
1	5	0	2.27634	39.558	0.338394	0.114510
-1	5	1	2.26615	39.743	0.339915	0.115542
1	0	3	2.26188	39.822	0.340556	0.115979
0	2	4	2.24561	40.123	0.343025	0.117666
1	1	3	2.23329	40.353	0.344917	0.118967
-1	0	4	2.19459	41.097	0.350999	0.123200
1	4	2	2.17709	41.442	0.353821	0.125189
-1	1	4	2.16845	41.615	0.355231	0.126189
1	5	1	2.16413	41.702	0.355939	0.126693
1	2	3	2.15361	41.915	0.357678	0.127934
-1	5	2	2.13817	42.232	0.360260	0.129787
-1	4	3	2.13357	42.328	0.361037	0.130348
0	3	4	2.11530	42.711	0.364157	0.132610
0	6	2	2.10410	42.950	0.366094	0.134024
0	5	3	2.10287	42.976	0.366309	0.134182
-1	2	4	2.09528	43.140	0.367635	0.135155
1	3	3	2.03787	44.419	0.377992	0.142878



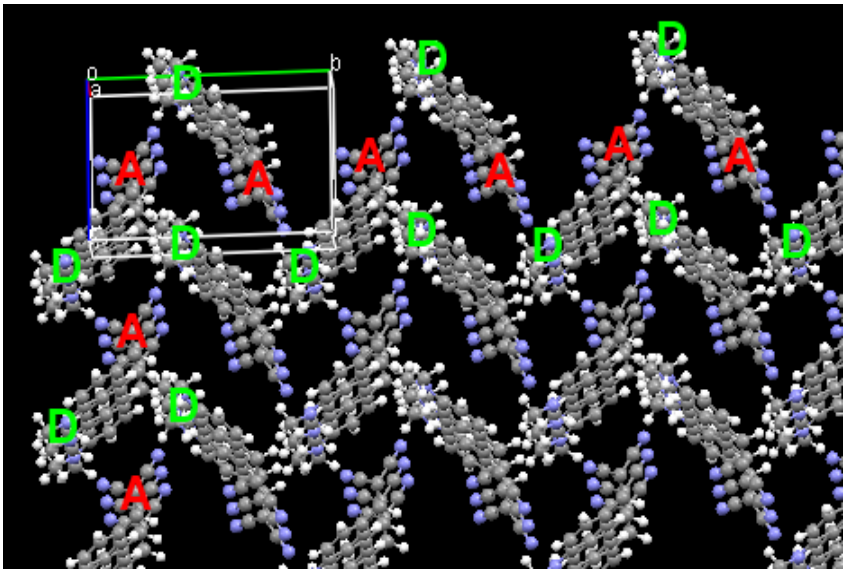


Figure S3-2 Crystal structure of the nanowires of compound 1.

Part S4

Molecule in figure S4a) (calculated dipole moment =12.11 debye) can form uniform semi-1-D nanostructures, whereas molecule in Figure S4b) (calculated dipole moment =6.28 debye) can only organize into nanoparticles. The two molecules are very similar except for the difference of the acceptor segments and hence the resulting dipole moment. This further supports that the molecular dipole moment has a crucial impact on the resulting morphology of nanostructures.

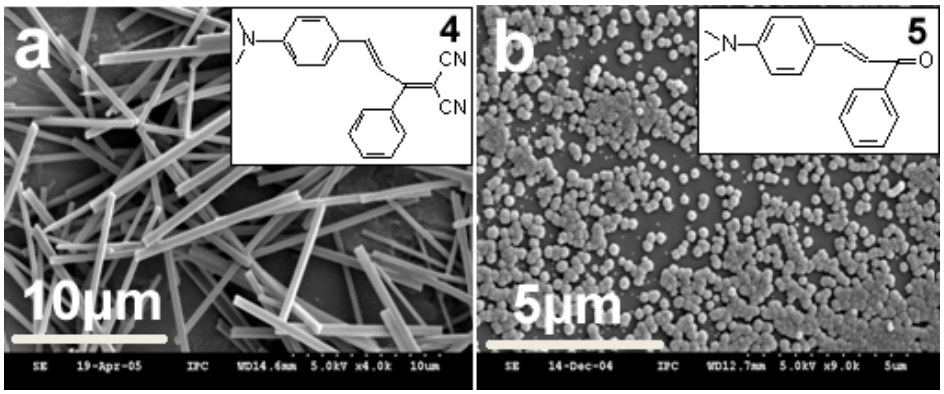


Figure S4, SEM images of the corresponding nanostructures obtained from the molecules whose structures are shown in the inset.

Part S5

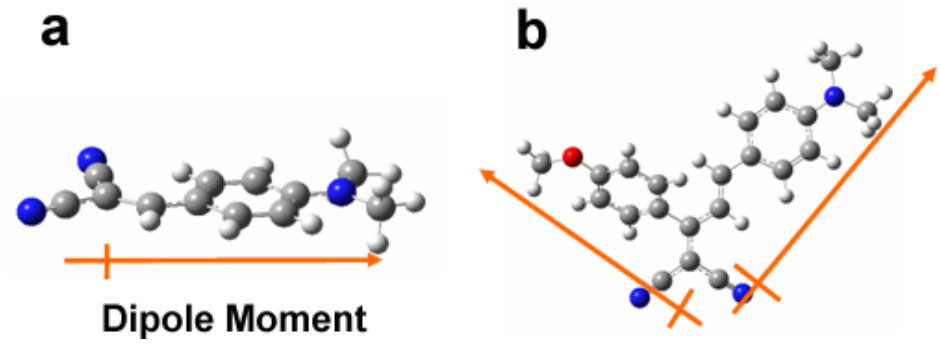


Figure S5 energy minimized molecular model a) for compound 1 with one dipole moment direction, b) for compound 6 with two dipole moment directions.

Part S6

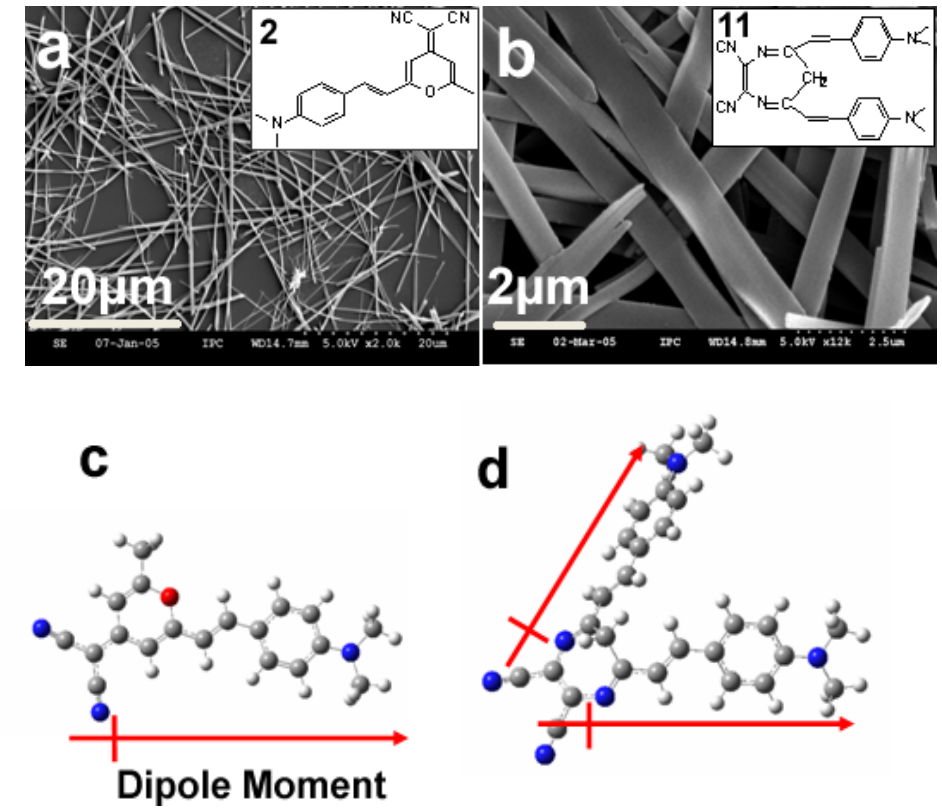


Figure S6, SEM images of organic nanostructures formed from a) D-A type compound 2 with a dipole moment in one direction: nanowires. and b) D-A-D type compound 11 with a dipole moment in two directions: nanoribbons. Inset in each image is the corresponding molecular structure. c), d) is the energy minimized molecular model for compound 2 and 11 respectively.

Part S7

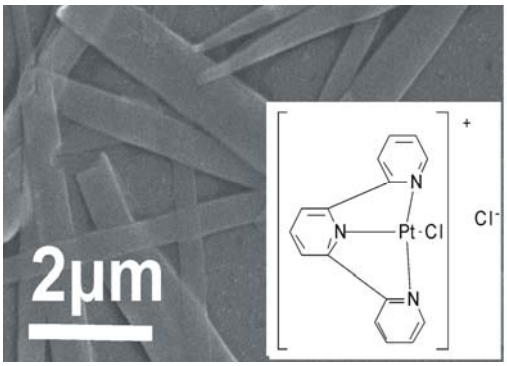


Figure S7-1 SEM image of nanostructures formed by using metal-metal (ligand) interactions as the driving force. Inset is the molecular structure.

1) L. S. Shimizu, A. D. Hughes, M. D. Smith, M. J. Davis, B. P. Zhang, H. C. Zur Loye, K. D. Shimizu, *J. Am. Chem. Soc*. **2003**, 125, 14972. 2) Y. Liu, Y. Li, L. Jiang, H. Gan, H. Liu, Y. Li, J. Zhuang, F. Lu, D. Zhu, *J. Org. Chem.* **2004**, 69, 9049. 3) Y, Liu, S. Xiao, H. Li, Y. Li, H. Liu, F. Lu, J. Zhuang, D. Zhu, *J. Phys. Chem. B* **2004**, 108, 6256.

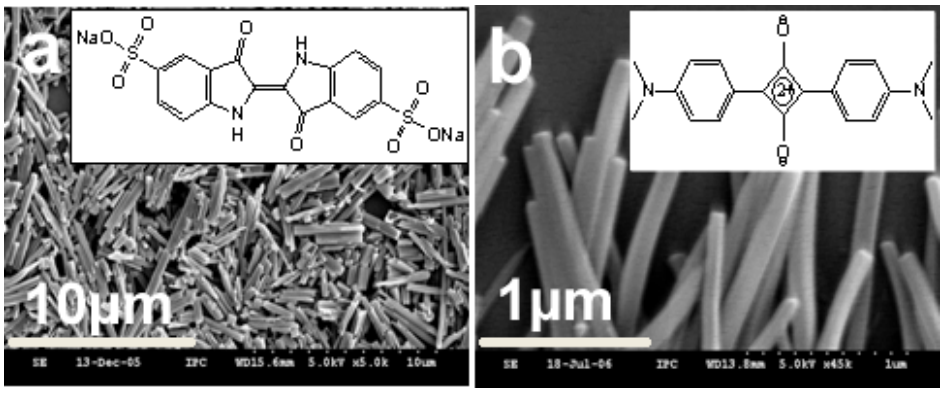


Figure S7-2 SEM images of nanostructures formed by the use of a) lowing the temperature of the solution and b) evaporation of the solvent method to gain supersaturation, nucleation process and then achieved the growth of 1-D nanostructures.

Indigo carmine (inset of Figure S7a) was first dissolved in water at 353 K to get a clear saturated solution. The temperature of the solution was then gradually decreased to room

temperature. Some precipitates would form at the bottom of the solution.

2,4-bis[4-(N,N-dimethylamino)phenyl] squaraine (inset of Figure S7b) was first dissolved in dichloromethane (CH_2Cl_2) to a concentration of 1×10^{-3} M. A few drops of the sample were placed on silicon substrates, and the solvent was left to evaporate. After evaporation, nanorods formed on the substrate;

Part S8

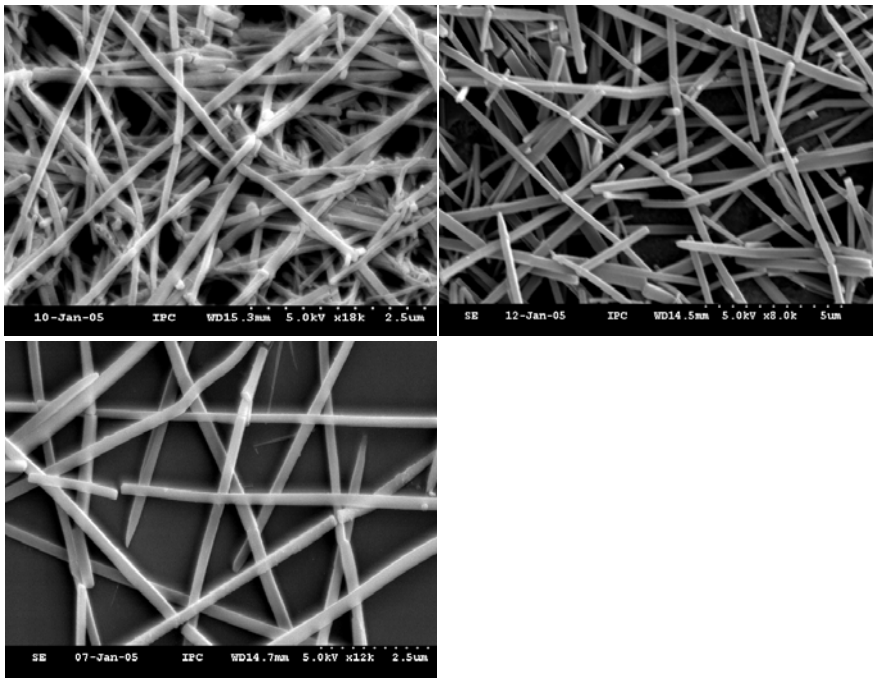


Figure S8. SEM images of nanowires formed at different concentrations of coumpound 2 a) 5×10^{-4}, b) 1×10^{-3} and c) 2×10^{-3} mol/L.