Electronic Supplementary Material (ESI) for RSC Advances

Molecular-dynamics simulation of polyimide matrix pre-crystallization near the surface of a single-walled carbon nanotube. Supporting information.

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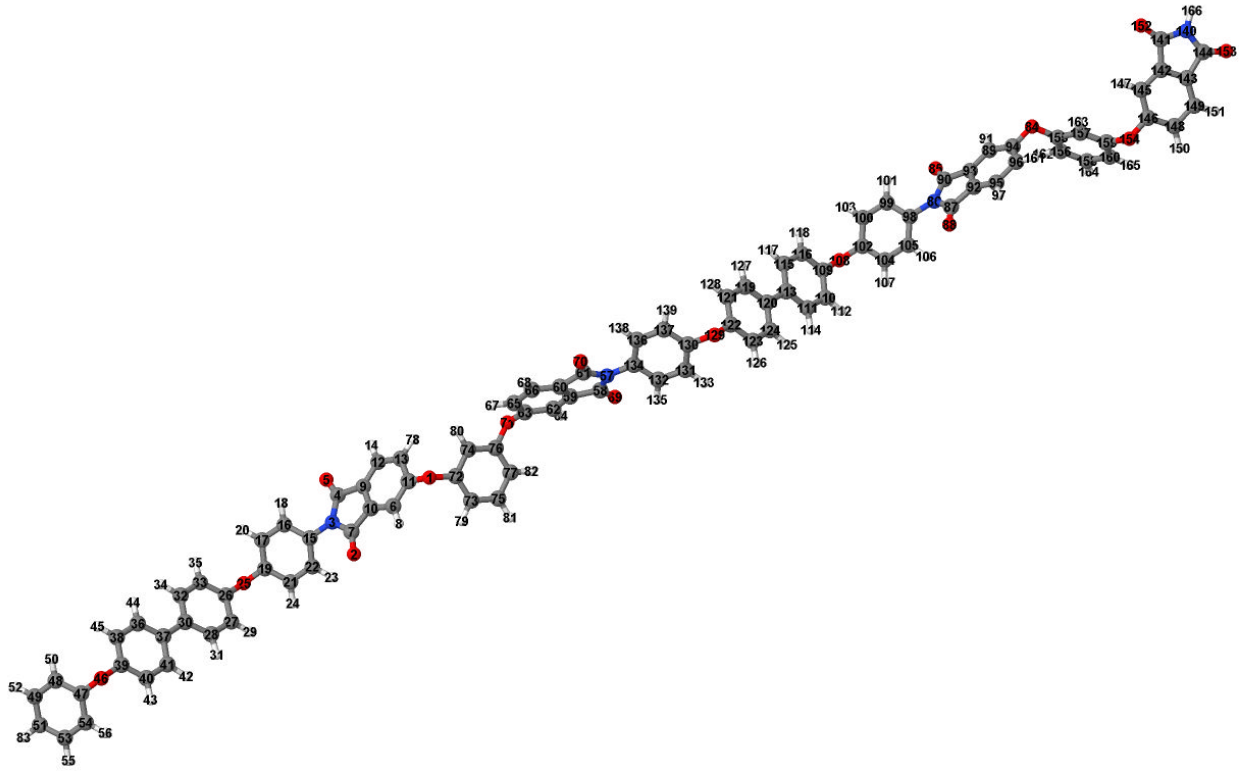

Fig. S.1. R-BAPB dimer configuration after geometry optimization using HF/6-31G* quantum mechanics method

Table S.1. Partial charges of the R-BAPB dimer fragment

Atom number	*Atom type*	*Partial charge*	*Atom number*	*Atom type*	*Partial charge*	*Atom number*	*Atom type*	*Partial charge*
1	O	-0.716	57	N	-0.928	113	C	-0.022
2	O	-0.548	58	C	0.852	114	H	0.163
3	N	-0.928	59	C	-0.138	115	C	-0.147
4	C	0.853	60	C	-0.176	116	C	-0.173
5	O	-0.554	61	C	0.853	117	H	0.165
6	C	-0.144	62	C	-0.144	118	H	0.175
7	C	0.852	63	C	0.397	119	C	-0.148
8	H	0.214	64	H	0.214	120	C	-0.022
9	C	-0.176	65	C	-0.207	121	C	-0.172
10	C	-0.138	66	C	-0.092	122	C	0.350
11	C	0.396	67	H	0.189	123	C	-0.163
12	C	-0.093	68	H	0.204	124	C	-0.147
13	C	-0.206	69	O	-0.548	125	H	0.163
14	H	0.204	70	O	-0.554	126	H	0.174
15	C	0.262	71	O	-0.716	127	H	0.165
16	C	-0.101	72	C	0.354	128	H	0.175

Atom number	*Atom type*	*Partial charge*	*Atom number*	*Atom type*	*Partial charge*	*Atom number*	*Atom type*	*Partial charge*
17	C	-0.215	73	C	-0.169	129	O	-0.720
18	H	0.176	74	C	-0.188	130	C	0.390
19	C	0.394	75	C	-0.145	131	C	-0.211
20	H	0.179	76	C	0.354	132	C	-0.102
21	C	-0.194	77	C	-0.169	133	H	0.178
22	C	-0.100	78	H	0.189	134	C	0.263
23	H	0.175	79	H	0.181	135	H	0.176
24	H	0.175	80	H	0.195	136	C	-0.101
25	O	-0.721	81	H	0.174	137	C	-0.194
26	C	0.345	82	H	0.18	138	H	0.177
27	C	-0.167	83	H	0.153	139	H	0.176
28	C	-0.15	84	O	-0.716	140	N	-0.816
29	H	0.173	85	O	-0.548	141	C	0.827
30	C	-0.016	86	N	-0.928	142	C	-0.143
31	H	0.163	87	C	0.854	143	C	-0.176
32	C	-0.149	88	O	-0.554	144	C	0.829
33	C	-0.164	89	C	-0.144	145	C	-0.160
34	H	0.163	90	C	0.852	146	C	0.395
35	H	0.173	91	H	0.215	147	H	0.216
36	C	-0.140	92	C	-0.176	148	C	-0.183
37	C	-0.034	93	C	-0.138	149	C	-0.092
38	C	-0.197	94	C	0.397	150	H	0.189
39	C	0.380	95	C	-0.092	151	H	0.204
40	C	-0.184	96	C	-0.207	152	O	-0.548
41	C	-0.138	97	H	0.204	153	O	-0.552
42	H	0.162	98	C	0.264	154	O	-0.717
43	H	0.171	99	C	-0.102	155	C	0.355
44	H	0.161	100	C	-0.194	156	C	-0.168
45	H	0.174	101	H	0.177	157	C	-0.185
46	O	-0.719	102	C	0.389	158	C	-0.143
47	C	0.357	103	H	0.176	159	C	0.352
48	C	-0.176	104	C	-0.209	160	C	-0.168
49	C	-0.145	105	C	-0.102	161	H	0.188
50	H	0.170	106	H	0.177	162	H	0.181
51	C	-0.158	107	H	0.178	163	H	0.194
52	H	0.157	108	O	-0.720	164	H	0.174
53	C	-0.145	109	C	0.352	165	H	0.180
54	C	-0.166	110	C	-0.164	166	H	0.340
55	H	0.157	111	C	-0.147			
56	H	0.169	112	H	0.175			

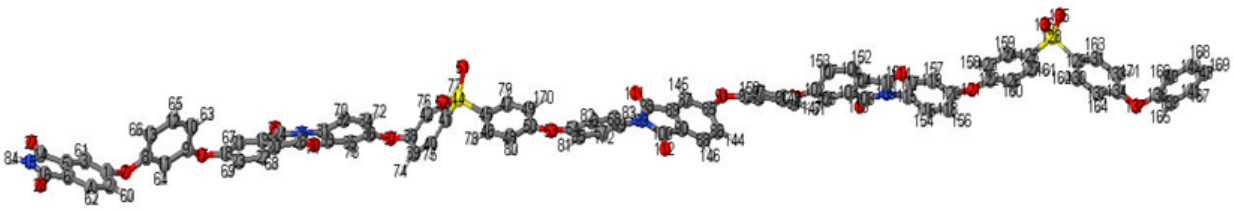

Fig. S.2. R-BAPS dimer configuration after geometry optimization using HF/6-31G* quantum mechanics method

Table S.2. Partial charges of the R-BAPB dimer fragment

Atom number	*Atom type*	*Partial charge*	*Atom number*	*Atom type*	*Partial charge*	*Atom number*	*Atom type*	*Partial charge*
1	C	0.433	59	C	0.293	117	C	-0.213
2	C	-0.272	60	H	-0.891	118	C	-0.253
3	C	-0.238	61	H	-0.289	119	C	-0.272
4	C	-0.166	62	H	0.241	120	C	0.406
5	C	-0.115	63	H	0.262	121	O	-0.718
6	C	-0.145	64	H	0.255	122	C	0.423
7	O	-0.725	65	H	0.230	123	C	-0.261
8	C	0.435	66	H	0.242	124	C	-0.158
9	C	0.442	67	H	0.221	125	C	-0.376
10	C	-0.255	68	H	0.232	126	C	-0.248
11	C	-0.328	69	H	0.268	127	C	-0.160
12	C	-0.182	70	H	0.261	128	S	1.58
13	C	-0.282	71	H	0.245	129	C	-0.316
14	C	0.85	72	H	0.276	130	C	-0.175
15	N	-0.807	73	H	0.273	131	C	-0.162
16	C	0.845	74	H	0.228	132	C	-0.250
17	O	-0.725	75	H	0.239	133	C	-0.269
18	C	0.440	76	H	0.244	134	C	0.431
19	C	-0.115	77	H	0.273	135	O	-0.698
20	C	-0.146	78	H	0.237	136	O	-0.682
21	C	-0.235	79	H	0.261	137	O	-0.718
22	C	-0.168	80	H	0.239	138	C	0.333
23	C	-0.271	81	H	0.252	139	C	-0.208
24	C	0.875	82	H	0.230	140	C	-0.218
25	N	-0.967	83	H	0.244	141	C	-0.251
26	C	0.872	84	H	0.225	142	C	-0.247
27	O	-0.560	85	C	0.433	143	C	0.293
28	O	-0.570	86	C	-0.272	144	H	-0.891
29	O	-0.557	87	C	-0.238	145	H	-0.289
30	O	-0.556	88	C	-0.166	146	H	0.241
31	C	0.317	89	C	-0.115	147	H	0.262
32	C	-0.217	90	C	-0.145	148	H	0.255
33	C	-0.213	91	O	-0.725	149	H	0.230
34	C	-0.253	92	C	0.435	150	H	0.242
35	C	-0.272	93	C	0.442	151	H	0.221
36	C	0.406	94	C	-0.255	152	H	0.232
37	O	-0.718	95	C	-0.328	153	H	0.268

Atom number	*Atom type*	*Partial charge*	*Atom number*	*Atom type*	*Partial charge*	*Atom number*	*Atom type*	*Partial charge*
38	C	0.423	96	C	-0.182	154	H	0.261
39	C	-0.261	97	C	-0.282	155	H	0.245
40	C	-0.158	98	C	0.85	156	H	0.276
41	C	-0.376	99	N	-0.807	157	H	0.273
42	C	-0.248	100	C	0.845	158	H	0.228
43	C	-0.160	101	O	-0.725	159	H	0.239
44	S	1.580	102	C	0.440	160	H	0.244
45	C	-0.316	103	C	-0.115	161	H	0.273
46	C	-0.175	104	C	-0.146	162	H	0.237
47	C	-0.162	105	C	-0.235	163	H	0.261
48	C	-0.250	106	C	-0.168	164	H	0.239
49	C	-0.269	107	C	-0.271	165	H	0.252
50	C	0.431	108	C	0.875	166	H	0.230
51	O	-0.698	109	N	-0.967	167	H	0.244
52	O	-0.682	110	C	0.872	168	H	0.225
53	O	-0.718	111	O	-0.56	169	H	0.226
54	C	0.333	112	O	-0.57	170	H	0.206
55	C	-0.208	113	O	-0.557	171	H	0.207
56	C	-0.218	114	O	-0.556	172	H	0.363
57	C	-0.251	115	C	0.317			
58	C	-0.247	116	C	-0.217			

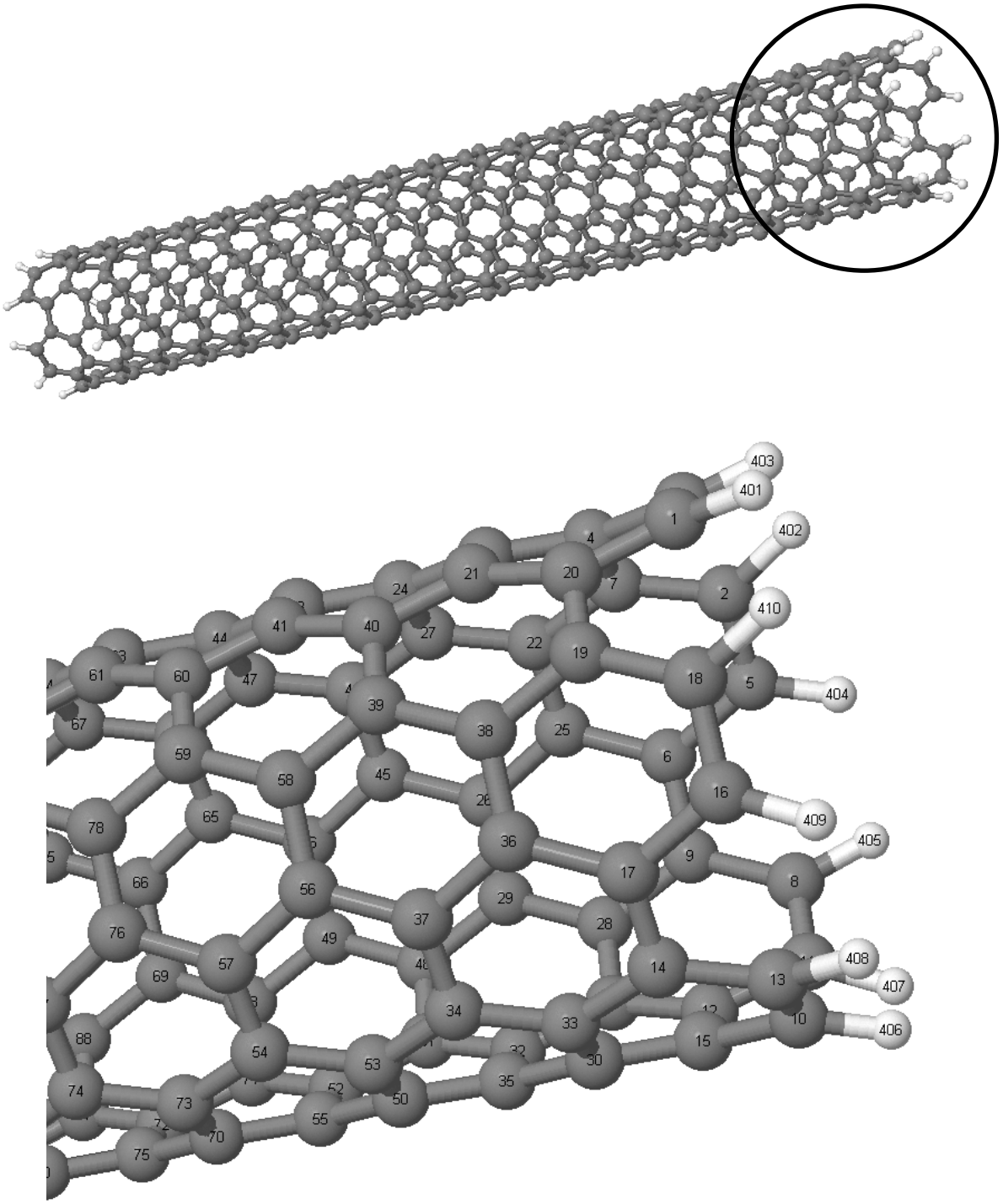

Fig. S.3. Configuration of carbon nanotube (CNT) with chirality (5,5). The lower pane shows increased one of the CNT end with atom numbers.

Table S.3. Partial charges of carbon nanotube. Atoms from 39 to 363 have the same zero charge.

Atom number	*Atom type*	*Partial charge*	*Atom number*	*Atom type*	*Partial charge*	*Atom number*	*Atom type*	*Partial charge*
1	C	-0.114	33	C	-0.013	389	C	-0.114
2	C	-0.114	34	C	0.000	390	C	-0.013
3	C	-0.114	35	C	0.000	391	C	-0.013
4	C	-0.013	36	C	-0.013	392	C	-0.114
5	C	-0.114	37	C	0.000	393	C	-0.013
6	C	-0.013	38	C	-0.013	394	C	-0.114
7	C	-0.013	**39-363**	**C**	**0.000**	395	C	-0.114
8	C	-0.114	364	C	-0.013	396	C	-0.013
9	C	-0.013	365	C	0.000	397	C	-0.114
10	C	-0.114	366	C	-0.013	398	C	-0.013
11	C	-0.114	367	C	-0.013	399	C	-0.114
12	C	-0.013	368	C	0.000	400	C	-0.114
13	C	-0.114	369	C	-0.013	401	H	0.140
14	C	-0.013	370	C	0.000	402	H	0.140
15	C	-0.013	371	C	0.000	403	H	0.140
16	C	-0.114	372	C	-0.013	404	H	0.140
17	C	-0.013	373	C	0.000	405	H	0.140
18	C	-0.114	374	C	-0.013	406	H	0.140
19	C	-0.013	375	C	-0.013	407	H	0.140
20	C	-0.013	376	C	0.000	408	H	0.140
21	C	-0.013	377	C	-0.013	409	H	0.140
22	C	-0.013	378	C	0.000	410	H	0.140
23	C	-0.013	379	C	-0.013	411	H	0.140
24	C	0.000	380	C	-0.013	412	H	0.140
25	C	-0.013	381	C	-0.013	413	H	0.140
26	C	0.000	382	C	-0.013	414	H	0.140
27	C	0.000	383	C	-0.013	415	H	0.140
28	C	-0.013	384	C	-0.114	416	H	0.140
29	C	0.000	385	C	-0.013	417	H	0.140
30	C	-0.013	386	C	-0.114	418	H	0.140
31	C	-0.013	387	C	-0.114	419	H	0.140
32	C	0.000	388	C	-0.013	420	H	0.140