

Supporting Information

Hybrid Nanotube-Graphene Junctions: Spin Degeneracy Breaking and Tunable Electronic Structure

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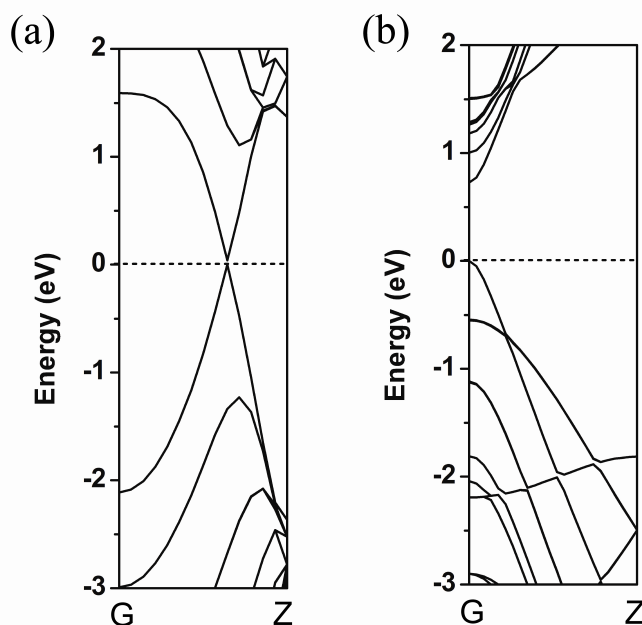


Figure S1. Electronic band structure of pristine (a) armchair CNT (6, 6) and (b) zig-zag CNT (10, 0).

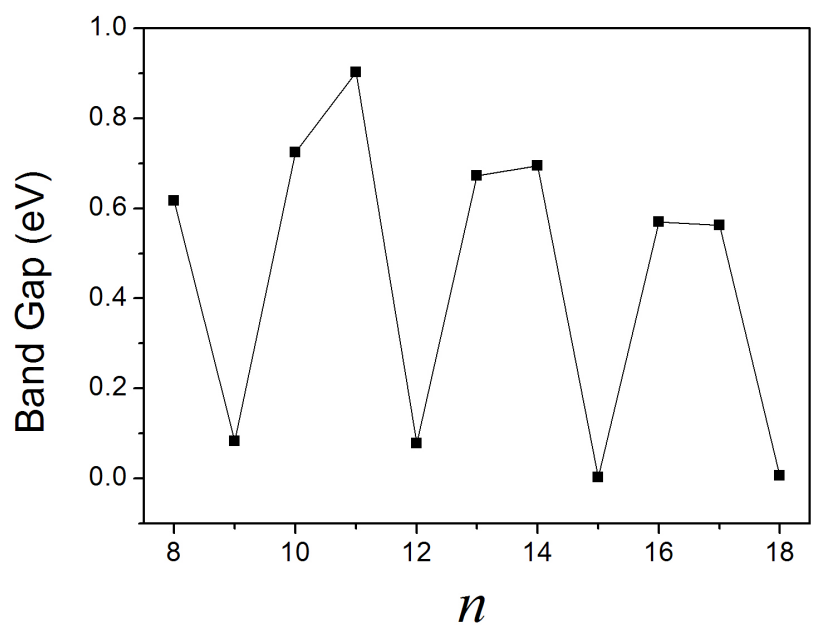


Figure S2. Band gap of zig-zag CNT (n , 0) as a function of n .

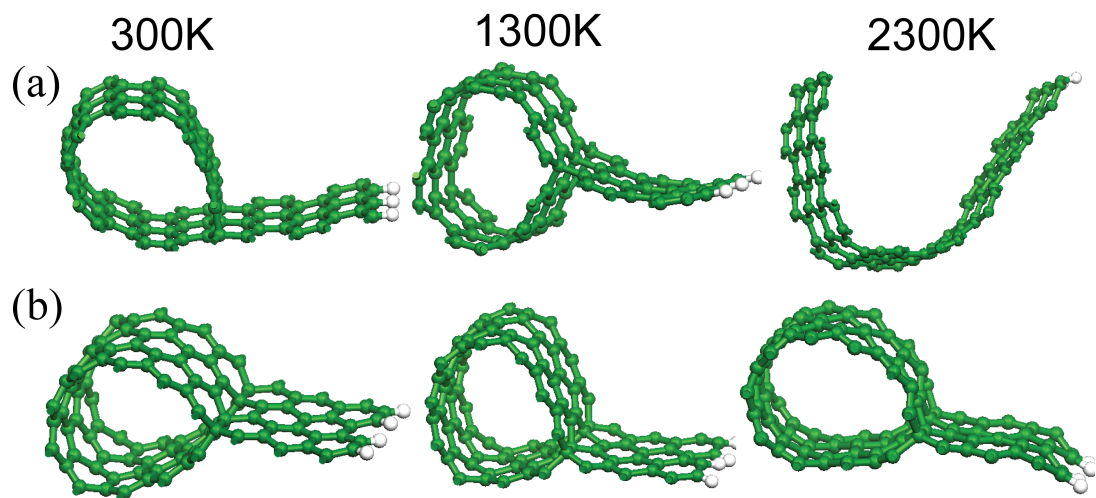


Figure S3. Geometric structure of (a) armchair NTGJ [(6, 6), 4] and (b) zig-zag NTGJ [(10, 0), 6] after 5 ps first-principles MD simulations at different temperatures.

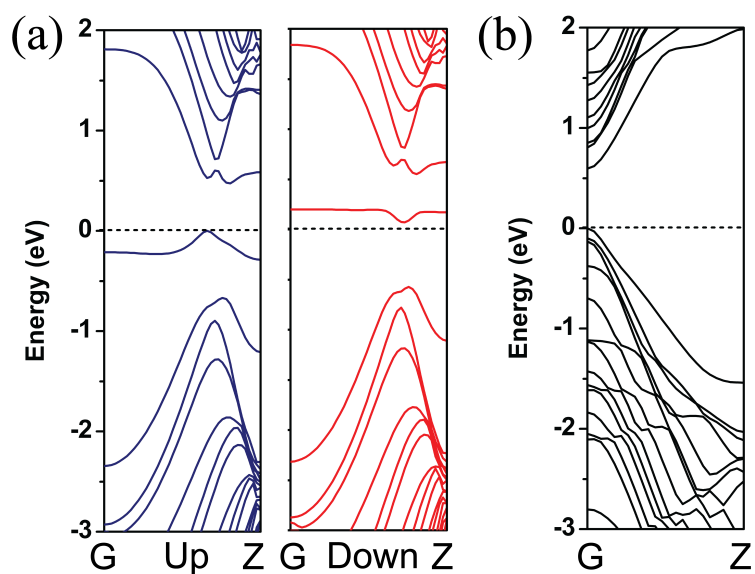


Figure S4. Electronic band structure for (a) armchair NTGJ [(6, 6), 4] and (b) zig-zag NTGJ [(10, 0), 6] from local density approximation (LDA) with PWC functional by DMol3 module.

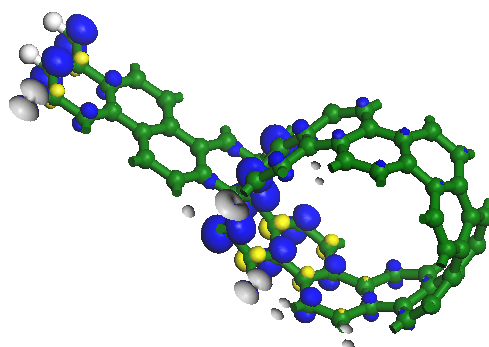


Figure S5. Computed spin density for armchair NTGJ [(6, 6), 4]. Blue and yellow represent spin-up and spin-down; the range of the iso-surface values of spin density is $[-0.03, 0.03]$ in atomic unit (a.u./bohr³).

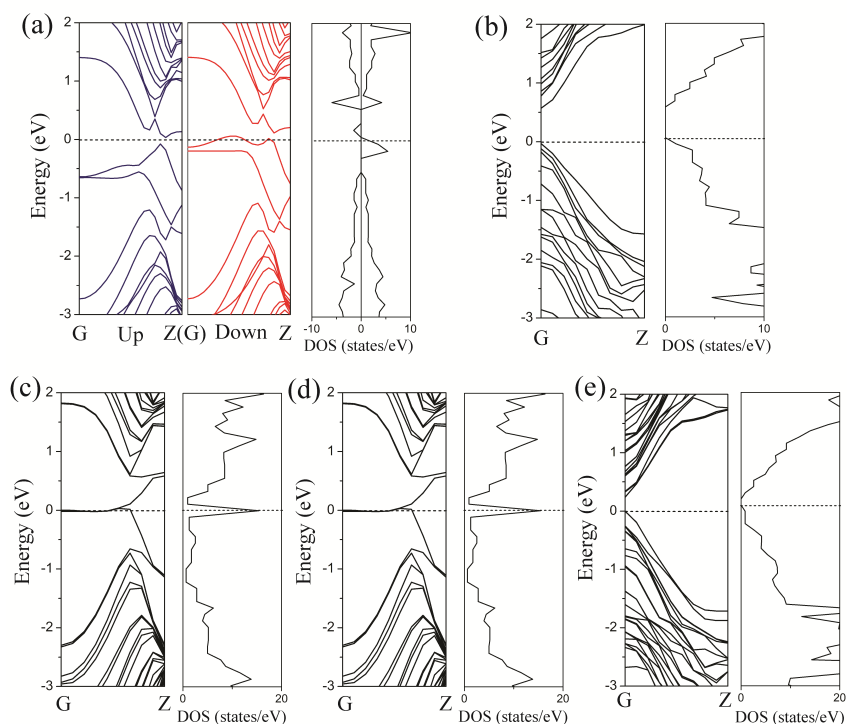


Figure S6. Electronic band structures and DOS plots for (a) armchair NTGJ [(6, 6), 4], (b) zig-zag NTGJ [(10, 0), 6], (c) cis- (d) trans-armchair dumbbell NTGJ [(6, 6), 4, (6, 6)] and (e) zig-zag dumbbell NTGJ [(10, 0), 6, (10, 0)] from VASP software.

Computational details of VASP is as follows: On the basis of optimized geometries by DMol³, the band structure and DOS calculations were performed using the Vienna ab initio Simulation Package (VASP 5.2) code based on density functional theory. The projector augmented wave (PAW) potentials were used to describe the interaction between ions and electrons. The nonlocal correlation energy was evaluated by vdW-DF2, Perdew-Burke-Ernzerhof (PBE) functional was used as the exchange functional. The electron wave function was expanded using plane waves with an energy cutoff of 400eV. A 1×1×8 Monkhorst-Pack k-point mesh was used to calculate DOS. Both $\Gamma(0\ 0\ 0)$ and $X(0\ 0\ 0.5)$ points are chosen as high symmetry k-points for band structure calculation, and 10 K points are calculated along each line. The obtained band structure and DOS were given in Figure S6.

Table S1. Atomic coordinates for armchair NTGJ [(6, 6), 4] and zig-zag NTGJ [(10, 0), 6] used in the calculations.

(a) Armchair NTGJ [(6, 6), 4]

No.	X	Y	Z	Atom
1	13.574	21.93	0.158	C
2	13.233	22.569	1.388	C
3	11.778	24.124	0.158	C
4	12.337	23.671	1.388	C
5	7.695	24.525	0.158	C
6	10.495	24.742	0.158	C
7	9.79	24.885	1.388	C
8	6.571	23.647	0.158	C
9	6.167	23.052	1.388	C
10	8.368	24.78	1.388	C
11	5.759	20.967	0.158	C
12	5.753	21.686	1.388	C
13	8.23	17.661	0.158	C
14	6.183	19.605	0.158	C
15	6.569	18.999	1.388	C
16	9.582	17.207	0.158	C
17	10.289	17.104	1.388	C
18	7.61	18.024	1.388	C
19	12.41	17.274	0.158	C
20	11.723	17.148	1.388	C
21	14.019	20.59	0.158	C
22	13.899	17.692	0.158	C
23	14.147	18.477	1.388	C
24	14.125	19.863	1.388	C
25	14.566	16.33	5.077	C
26	14.846	15.691	3.847	C
27	15.43	14.383	3.847	C
28	15.724	13.736	5.077	C
29	16.314	12.437	5.077	C
30	16.608	11.791	3.847	C
31	17.203	10.48	3.847	C
32	17.486	9.856	5.077	C
33	17.937	8.862	0.158	H

(b) Zig-zag NTGJ [(10, 0), 6]:

No.	X	Y	Z	Atom
1	19.592	14.896	1.369	C
2	19.592	14.896	2.794	C
3	19.361	16.109	3.5	C
4	19.361	16.109	0.664	C
5	18.705	17.165	1.373	C
6	18.705	17.165	2.79	C

7	17.705	17.904	3.499	C
8	17.705	17.904	0.664	C
9	16.517	18.24	1.369	C
10	16.517	18.24	2.794	C
11	15.278	18.153	3.503	C
12	15.278	18.153	0.66	C
13	14.136	17.663	1.369	C
14	14.136	17.663	2.794	C
15	13.193	16.867	3.498	C
16	13.193	16.867	0.666	C
17	12.477	15.857	1.372	C
18	12.477	15.857	2.791	C
19	12.005	14.707	3.5	C
20	12.005	14.707	0.663	C
21	11.766	13.497	1.364	C
22	11.766	13.497	2.799	C
23	11.704	12.287	3.517	C
24	11.704	12.287	0.646	C
25	11.94	10.905	1.296	C
26	11.94	10.905	2.867	C
27	13.295	10.545	3.517	C
28	13.295	10.545	0.646	C
29	14.507	10.508	1.364	C
30	14.507	10.508	2.799	C
31	15.732	10.656	3.5	C
32	15.732	10.656	0.663	C
33	16.914	11.037	1.373	C
34	16.914	11.037	2.791	C
35	17.971	11.683	3.498	C
36	17.971	11.683	0.666	C
37	18.828	12.569	1.369	C
38	18.828	12.569	2.794	C
39	19.405	13.669	3.503	C
40	19.405	13.669	0.66	C
41	6.342	5.924	2.769	C
42	6.342	5.924	1.395	C
43	7.246	6.72	0.676	C
44	7.246	6.72	3.488	C
45	8.167	7.531	2.794	C
46	8.167	7.531	1.37	C
47	9.1	8.356	0.661	C
48	9.1	8.356	3.502	C
49	10.019	9.173	2.805	C
50	10.019	9.173	1.359	C
51	10.916	9.974	0.649	C
52	10.916	9.974	3.514	C
53	5.621	5.297	3.285	H
54	5.621	5.297	0.878	H

Table S2. Atomic coordinates for (a) *cis*- (b) *trans*-armchair dumbbell NTGJ [(6, 6), 4, (6, 6)] and (c) zig-zag dumbbell NTGJ [(10, 0), 6, (10, 0)].

(a) *cis*-armchair dumbbell NTGJ [(6, 6), 4, (6, 6)]

No.	X	Y	Z	Atom
1	11.094	23.687	0.166	C
2	10.358	23.653	1.396	C
3	8.341	22.977	0.166	C
4	8.995	23.3	1.396	C
5	6.273	19.437	0.166	C
6	7.252	22.075	0.166	C
7	6.821	21.488	1.396	C
8	6.598	18.063	0.166	C
9	6.972	17.439	1.396	C
10	6.327	20.165	1.396	C
11	8.696	16.2	0.166	C
12	8.032	16.501	1.396	C
13	12.737	17.033	0.166	C
14	10.097	16.004	0.166	C
15	10.821	16.101	1.396	C
16	13.713	18.067	0.166	C
17	14.108	18.667	1.396	C
18	12.14	16.619	1.396	C
19	14.855	20.653	0.166	C
20	14.675	19.984	1.396	C
21	12.487	23.526	0.166	C
22	15.083	22.198	0.166	C
23	14.463	22.765	1.396	C
24	13.197	23.305	1.396	C
25	16.608	22.253	5.085	C
26	17.308	22.244	3.855	C
27	18.743	22.228	3.855	C
28	19.459	22.222	5.085	C
29	20.886	22.217	5.085	C
30	21.602	22.216	3.855	C
31	29.278	23.696	2.625	C
32	30.013	23.65	1.396	C
33	32.029	22.961	2.625	C
34	31.378	23.29	1.396	C
35	34.089	19.408	2.625	C
36	33.113	22.052	2.625	C
37	33.542	21.463	1.396	C

38	33.763	18.034	2.625	C
39	33.387	17.41	1.396	C
40	34.036	20.138	1.396	C
41	31.66	16.166	2.625	C
42	32.326	16.469	1.396	C
43	27.627	17.027	2.625	C
44	30.259	15.975	2.625	C
45	29.533	16.076	1.396	C
46	26.663	18.074	2.625	C
47	26.277	18.68	1.396	C
48	28.218	16.606	1.396	C
49	25.549	20.686	2.625	C
50	25.729	20.008	1.396	C
51	27.877	23.538	2.625	C
52	25.276	22.225	2.625	C
53	25.899	22.757	1.396	C
54	27.165	23.331	1.396	C
55	23.042	22.226	1.396	C
56	23.745	22.234	2.625	C

(b) *trans*-armchair dumbbell NTGJ [(6, 6), 4, (6, 6)]

No.	X	Y	Z	Atom
1	28.43	19.434	0.185	C
2	29.153	19.491	1.415	C
3	31.148	20.233	0.185	C
4	30.513	19.891	1.415	C
5	33.083	23.85	0.185	C
6	32.211	21.18	0.185	C
7	32.611	21.779	1.415	C
8	32.715	25.226	0.185	C
9	32.328	25.834	1.415	C
10	33.059	23.131	1.415	C
11	30.572	27.03	0.185	C
12	31.234	26.75	1.415	C
13	26.567	26.056	0.185	C
14	29.153	27.185	0.185	C
15	28.444	27.064	1.415	C
16	25.627	24.981	0.185	C
17	25.264	24.365	1.415	C
18	27.14	26.485	1.415	C
19	24.602	22.343	0.185	C
20	24.756	23.022	1.415	C
21	27.026	19.557	0.185	C
22	24.407	20.803	0.185	C

23	25.037	20.274	1.415	C
24	26.316	19.75	1.415	C
25	22.892	20.721	2.645	C
26	22.194	20.718	1.415	C
27	10.286	22.186	0.185	C
28	9.562	22.157	1.415	C
29	7.538	21.498	0.185	C
30	8.185	21.817	1.415	C
31	5.507	17.937	0.185	C
32	6.447	20.584	0.185	C
33	6.032	19.996	1.415	C
34	5.836	16.55	0.185	C
35	6.204	15.93	1.415	C
36	5.55	18.655	1.415	C
37	7.921	14.678	0.185	C
38	7.269	14.98	1.415	C
39	11.964	15.497	0.185	C
40	9.334	14.476	0.185	C
41	10.046	14.568	1.415	C
42	12.938	16.542	0.185	C
43	13.318	17.147	1.415	C
44	11.374	15.091	1.415	C
45	14.031	19.151	0.185	C
46	13.861	18.476	1.415	C
47	11.685	22.014	0.185	C
48	14.265	20.685	0.185	C
49	13.65	21.231	1.415	C
50	12.389	21.798	1.415	C
51	15.783	20.733	5.104	C
52	16.48	20.724	3.874	C
53	17.914	20.713	3.874	C
54	18.624	20.712	5.104	C
55	20.051	20.711	5.104	C
56	20.761	20.713	3.874	C

(c) Zig-zag dumbbell NTGJ [(10, 0), 6, (10, 0)].

No.	X	Y	Z	Atom
1	33.351	17.969	1.418	C
2	33.351	17.969	2.844	C
3	34.007	19.017	3.549	C
4	34.007	19.017	0.713	C
5	34.241	20.238	1.423	C
6	34.241	20.238	2.839	C
7	33.997	21.457	3.549	C

8	33.997	21.457	0.713	C
9	33.333	22.499	1.418	C
10	33.333	22.499	2.844	C
11	32.351	23.26	3.552	C
12	32.351	23.26	0.71	C
13	31.174	23.654	1.419	C
14	31.174	23.654	2.843	C
15	29.941	23.698	3.547	C
16	29.941	23.698	0.715	C
17	28.729	23.444	1.422	C
18	28.729	23.444	2.84	C
19	27.6	22.927	3.549	C
20	27.6	22.927	0.713	C
21	26.597	22.207	1.413	C
22	26.597	22.207	2.849	C
23	25.725	21.365	3.566	C
24	25.725	21.365	0.696	C
25	24.967	20.185	1.346	C
26	24.967	20.185	2.916	C
27	25.73	19.009	3.566	C
28	25.73	19.009	0.696	C
29	26.611	18.176	1.413	C
30	26.611	18.176	2.849	C
31	27.623	17.469	3.549	C
32	27.623	17.469	0.713	C
33	28.759	16.967	1.422	C
34	28.759	16.967	2.84	C
35	29.974	16.728	3.547	C
36	29.974	16.728	0.715	C
37	31.207	16.787	1.419	C
38	31.207	16.787	2.843	C
39	32.378	17.198	3.552	C
40	32.378	17.198	0.71	C
41	17.473	20.205	2.828	C
42	17.473	20.205	1.434	C
43	18.677	20.202	0.723	C
44	18.677	20.202	3.539	C
45	19.907	20.197	2.841	C
46	19.907	20.197	1.421	C
47	21.149	20.192	0.711	C
48	21.149	20.192	3.551	C
49	22.379	20.188	2.853	C
50	22.379	20.188	1.409	C
51	23.583	20.184	0.698	C
52	23.583	20.184	3.564	C
53	7.705	22.42	3.548	C
54	7.705	22.42	4.974	C
55	7.049	21.372	5.679	C

56	7.049	21.372	2.843	C
57	6.816	20.151	3.553	C
58	6.816	20.151	4.969	C
59	7.059	18.933	5.679	C
60	7.059	18.933	2.843	C
61	7.723	17.89	3.548	C
62	7.723	17.89	4.974	C
63	8.705	17.13	5.682	C
64	8.705	17.13	2.84	C
65	9.882	16.735	3.549	C
66	9.882	16.735	4.973	C
67	11.115	16.691	5.677	C
68	11.115	16.691	2.845	C
69	12.327	16.945	3.552	C
70	12.327	16.945	4.97	C
71	13.456	17.462	5.679	C
72	13.456	17.462	2.843	C
73	14.459	18.182	3.543	C
74	14.459	18.182	4.979	C
75	15.331	19.024	5.696	C
76	15.331	19.024	2.826	C
77	16.089	20.204	3.476	C
78	16.089	20.204	5.046	C
79	15.326	21.38	5.696	C
80	15.326	21.38	2.826	C
81	14.445	22.213	3.543	C
82	14.445	22.213	4.979	C
83	13.433	22.92	5.679	C
84	13.433	22.92	2.843	C
85	12.297	23.422	3.552	C
86	12.297	23.422	4.97	C
87	11.082	23.661	5.677	C
88	11.082	23.661	2.845	C
89	9.849	23.602	3.549	C
90	9.849	23.602	4.973	C
91	8.678	23.191	5.682	C
92	8.678	23.191	2.84	C
