Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting information for:

Electronic Properties of Carbon Nanotubes Complexed with a DNA Nucleotide

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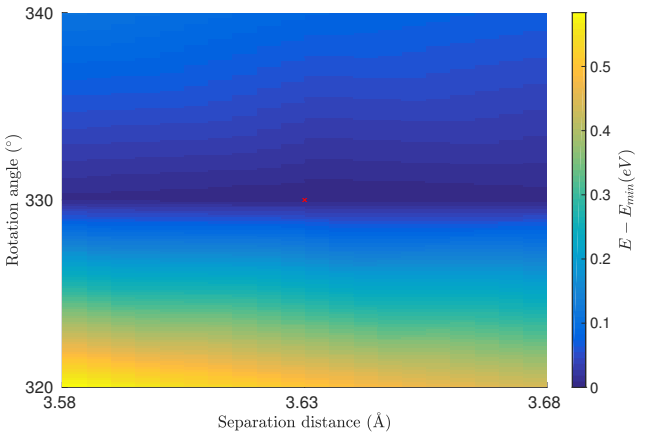
Table S1: Binding energies (kcal/mol) for S66 data set

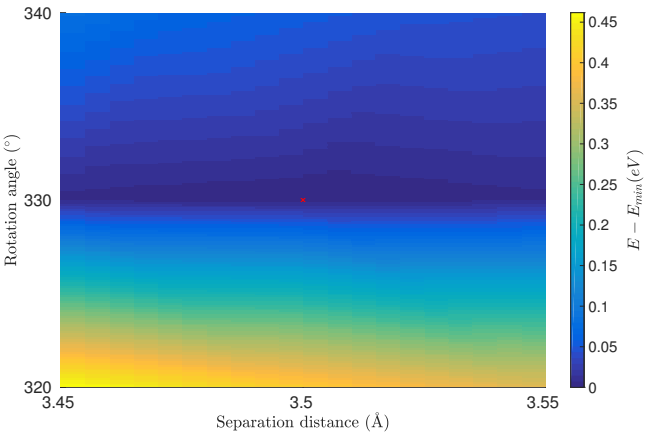
No.	DFTB3	DFTB3-UFF	DFTB3-SK	DFTB3-D3	CCSD(T)[S1]
1	-4.400	-3.759	-4.423	-4.860	-4.918
2	-4.331	-3.655	-4.414	-5.098	-5.592
3	-3.920	-3.369	-4.082	-4.732	-6.908
4	-7.356	-6.328	-7.541	-8.475	-8.103
5	-3.867	-3.572	-4.105	-4.845	-5.757
6	-3.466	-3.524	-4.089	-4.848	-7.554
7	-6.335	-5.940	-6.948	-7.850	-8.23
8	-3.812	-3.364	-3.886	-4.403	-5.009
9	-1.188	-1.840	-1.836	-2.329	-3.059
10	-0.563	-0.761	-1.390	-2.040	-4.16
11	-1.983	-2.523	-3.228	-4.073	-5.419
12	-3.381	-2.495	-3.510	-4.348	-7.266
13	-3.441	-4.130	-4.243	-5.032	-6.187
14	-2.714	-3.648	-4.075	-4.664	-7.454
15	-5.532	-6.939	-7.144	-7.917	-8.63
16	-3.618	-3.671	-3.856	-4.439	-5.124
17	-12.861	-12.165	-14.099	-15.148	-17.182
18	-3.298	-2.915	-3.487	-4.257	-6.857
19	-2.977	-3.065	-3.570	-4.351	-7.41
20	-17.374	-15.342	-17.748	-19.150	-19.093
21	-13.611	-12.368	-14.480	-15.468	-16.265
22	-16.415	-14.946	-17.120	-18.425	-19.491
23	-15.439	-14.316	-16.498	-17.542	-19.189

24	0.433	-4.165	-2.908	-3.380	-2.822
25	0.136	-4.183	-3.344	-3.909	-3.895
26	-3.155	-6.985	-7.407	-9.258	-9.829
27	0.274	-4.165	-3.136	-3.684	-3.439
28	-0.948	-5.555	-4.893	-6.066	-5.713
29	-1.773	-5.862	-5.624	-6.823	-6.819
30	0.330	-2.244	-1.612	-1.901	-1.432
31	-0.844	-3.180	-2.876	-3.612	-3.38
32	-1.478	-3.053	-3.371	-3.858	-3.738
33	0.249	-2.147	-1.660	-2.064	-1.872
34	-0.265	-5.357	-3.600	-4.728	-3.776
35	-0.394	-3.994	-2.839	-3.510	-2.613
36	-0.475	-3.418	-2.412	-2.747	-1.777
37	-0.420	-3.888	-2.733	-3.394	-2.404
38	-0.254	-4.107	-2.949	-3.680	-2.997
39	0.071	-4.255	-2.892	-3.729	-3.575
40	-0.201	-3.842	-2.497	-3.251	-2.895
41	-0.655	-5.463	-4.227	-5.614	-4.848
42	-0.385	-4.663	-3.736	-4.711	-4.138
43	-0.203	-3.886	-2.786	-3.797	-3.712
44	-0.175	-2.454	-1.653	-2.462	-2.005
45	-0.062	-2.170	-1.651	-1.944	-1.748
46	-0.537	-4.476	-3.471	-4.721	-4.264
47	-0.120	-2.447	-1.879	-2.711	-2.876
48	-0.371	-2.375	-2.041	-2.982	-3.535

49	-0.217	-2.387	-1.979	-2.848	-3.331
50	-0.853	-1.460	-1.958	-2.544	-2.867
51	-0.662	-0.775	-1.086	-1.295	-1.524
52	-2.304	-2.779	-3.164	-4.615	-4.707
53	-1.709	-2.726	-2.943	-3.791	-4.361
54	-1.697	-2.022	-2.089	-3.220	-3.277
55	-1.363	-2.477	-2.477	-3.802	-4.188
56	-0.353	-2.092	-2.202	-2.865	-3.231
57	-1.275	-3.780	-3.817	-4.804	-5.282
58	-0.440	-0.609	-1.342	-1.978	-4.146
59	-2.334	-2.108	-2.435	-2.743	-2.85
60	-3.007	-2.235	-3.383	-4.261	-4.868
61	-0.496	-3.524	-2.338	-3.519	-2.912
62	-0.828	-3.978	-3.185	-4.155	-3.534
63	-0.766	-3.325	-2.624	-3.783	-3.801
64	-0.851	-2.440	-2.135	-2.942	-2.999
65	-1.849	-2.043	-2.391	-2.745	-3.991
66	-0.272	-1.492	-1.743	-2.573	-3.968


Rotation angle (°)
340
330
320
3.58
3.63
3.68
Separation distance (Å)
0.5
0.4
0.3
0.2
0.1
0
$E - E_{min}(eV)$

(a)


Rotation angle (°)
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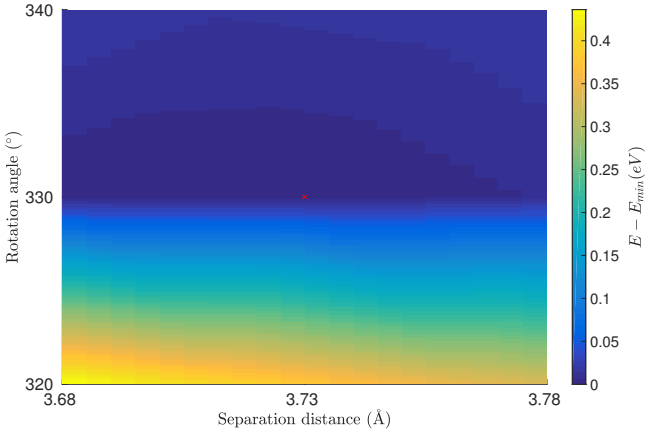
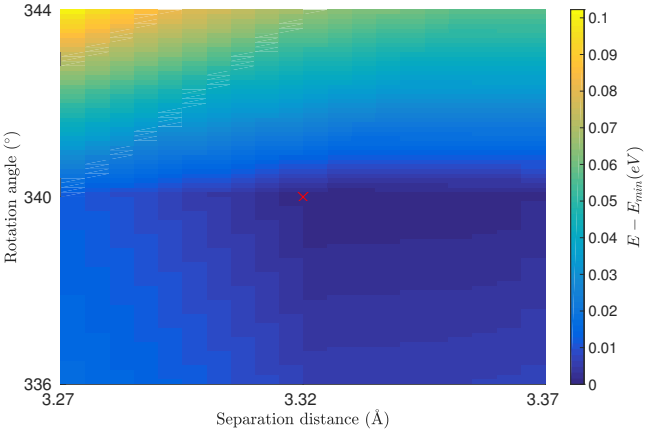
330
320
3.45
3.5
3.55
Separation distance (Å)
0.45
0.4
0.35
0.3
0.25
0.2
0.15
0.1
0.05
0
$E - E_{min}(eV)$

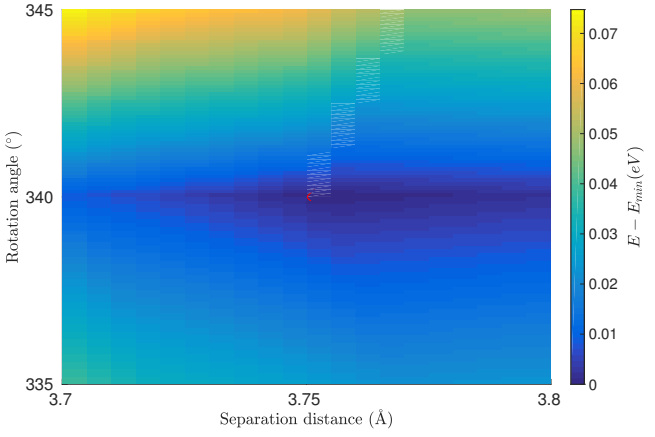
(b)


Rotation angle (°)
340
330
320
3.68
3.73
3.78
Separation distance (Å)
0.4
0.35
0.3
0.25
0.2
0.15
0.1
0.05
0
$E - E_{min}(eV)$

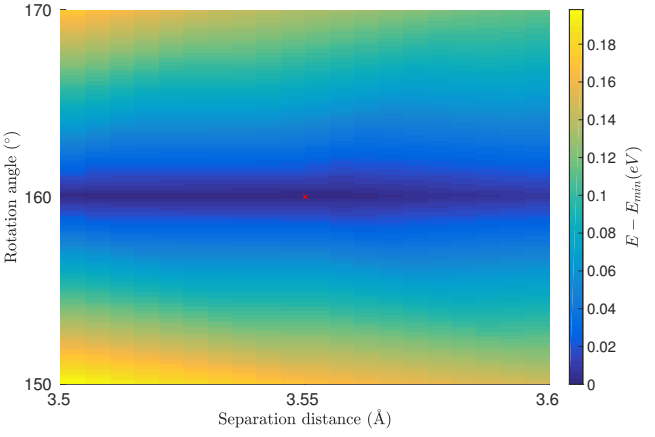
(c)


Rotation angle (°)
344
340
336
3.27
3.32
3.37
Separation distance (Å)
0.1
0.09
0.08
0.07
0.06
0.05
0.04
0.03
0.02
0.01
0
$E - E_{min}(eV)$

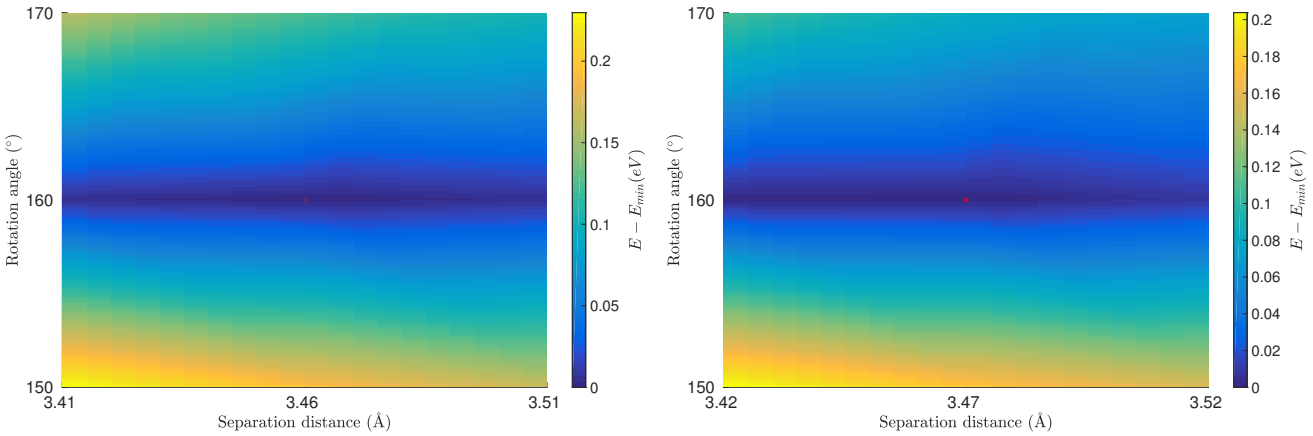
(d)


Rotation angle (°)
345
340
335
3.7
3.75
3.8
Separation distance (Å)
0.07
0.06
0.05
0.04
0.03
0.02
0.01
0
$E - E_{min}(eV)$

(e)

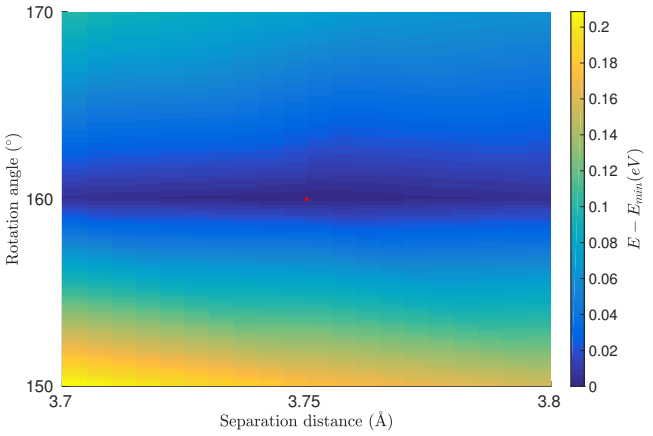

Rotation angle (°)
170
160
150
3.5
3.55
3.6
Separation distance (Å)
0.18
0.16
0.14
0.12
0.1
0.08
0.06
0.04
0.02
0
$E - E_{min}(eV)$

(f)

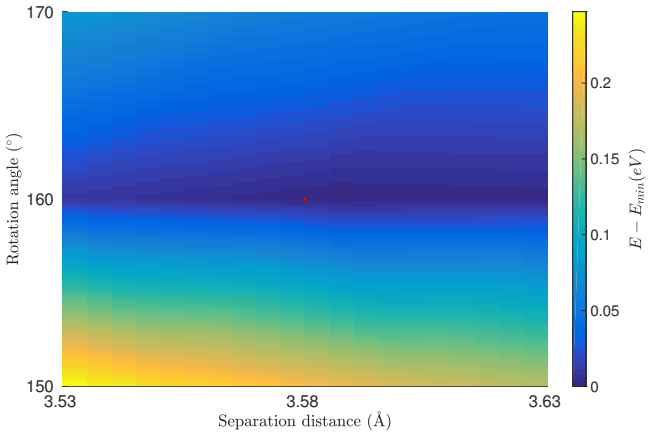


(g)

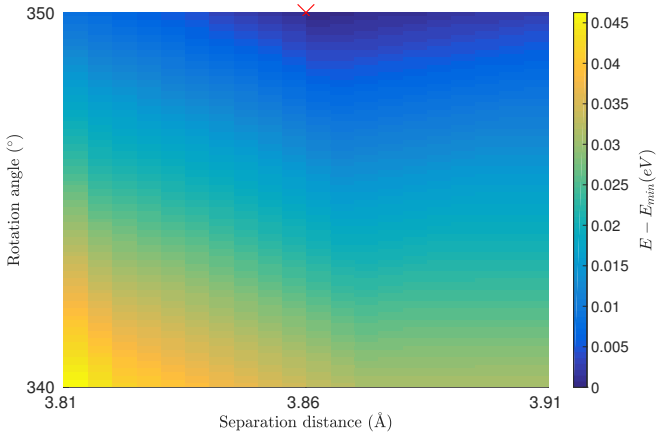
(h)



(i)



(j)



(k)

Figure S1: 2-D potential energy map for the complexes of AMP with : (a) (5,0) CNT, (b) (6,0) CNT, (c) (7,0) CNT, (d) (8,0) CNT, (e) (9,0) CNT, (f) (10,0) CNT, (g) (11,0) CNT, (h) (12,0) CNT, (i) (13,0) CNT, (j) (14,0) CNT, and (k) (15,0) CNT, all in vacuum. The red colored × symbol represents the minimum energy.

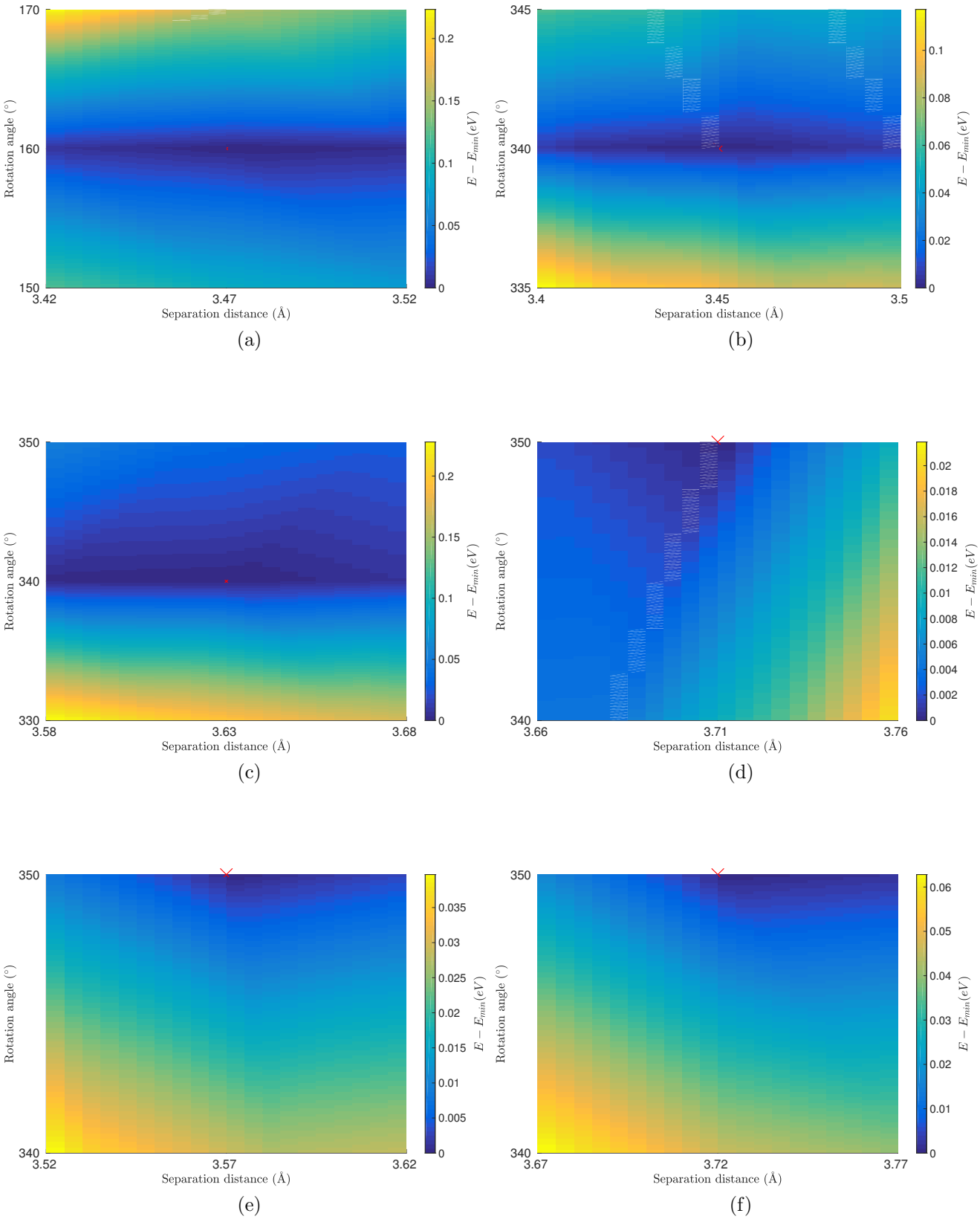
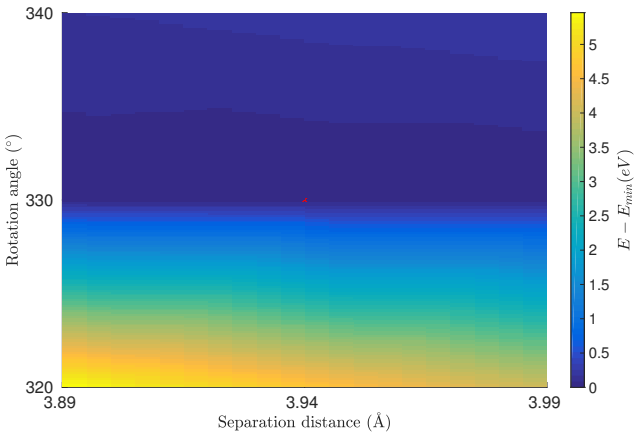
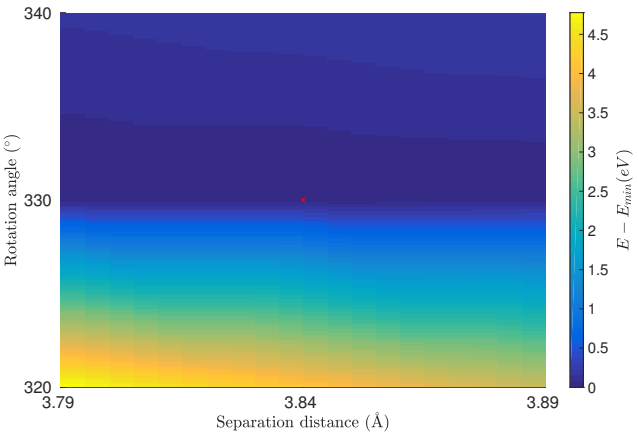


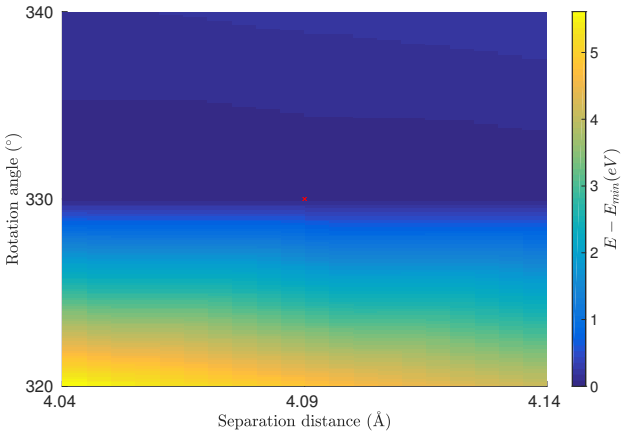
Figure S2: 2-D potential energy map for the complexes of AMP with : (a) (5,5) CNT, (b) (6,6) CNT, (c) (7,7) CNT, (d) (8,8) CNT, (e) (9,9) CNT, and (f) (10,10) CNT, all in vacuum. The red colored × symbol represents the minimum energy.


Rotation angle (°)
340
330
320
3.89
3.94
3.99
Separation distance (Å)
$E - E_{min}(eV)$
0
0.5
1
1.5
2
2.5
3
3.5
4
4.5
5

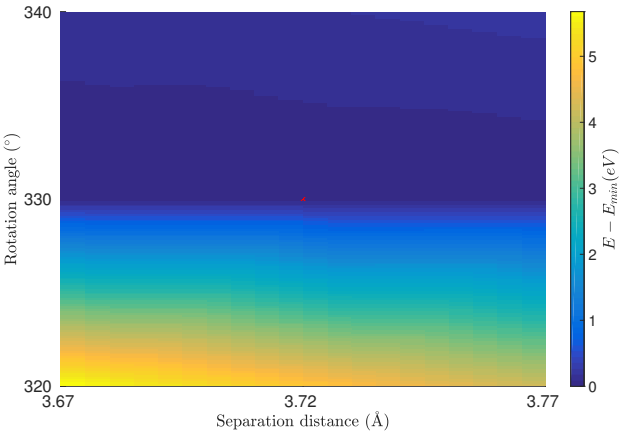
(a)


Rotation angle (°)
340
330
320
3.79
3.84
3.89
Separation distance (Å)
$E - E_{min}(eV)$
0
0.5
1
1.5
2
2.5
3
3.5
4
4.5

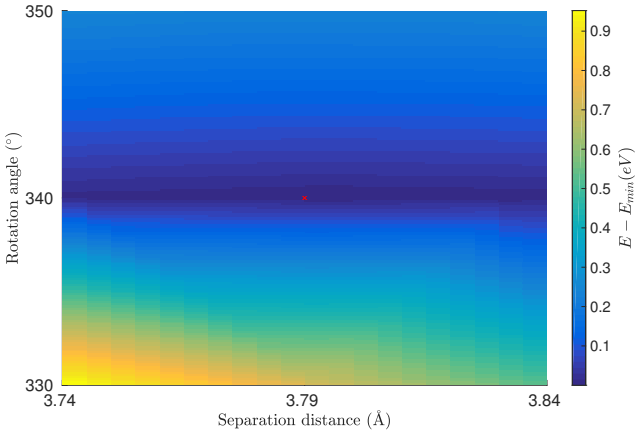
(b)


Rotation angle (°)
340
330
320
4.04
4.09
4.14
Separation distance (Å)
$E - E_{min}(eV)$
0
1
2
3
4
5

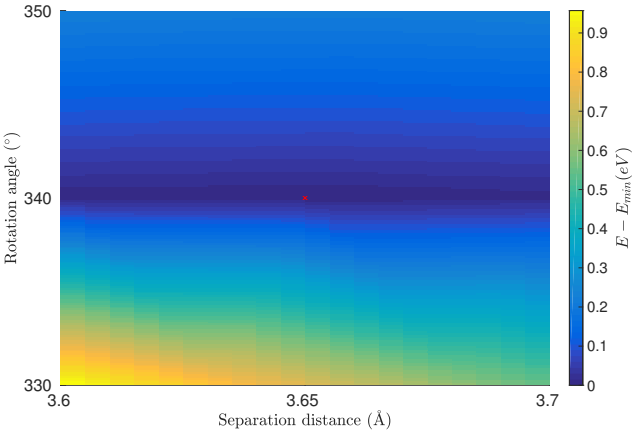
(c)


Rotation angle (°)
340
330
320
3.67
3.72
3.77
Separation distance (Å)
$E - E_{min}(eV)$
0
1
2
3
4
5

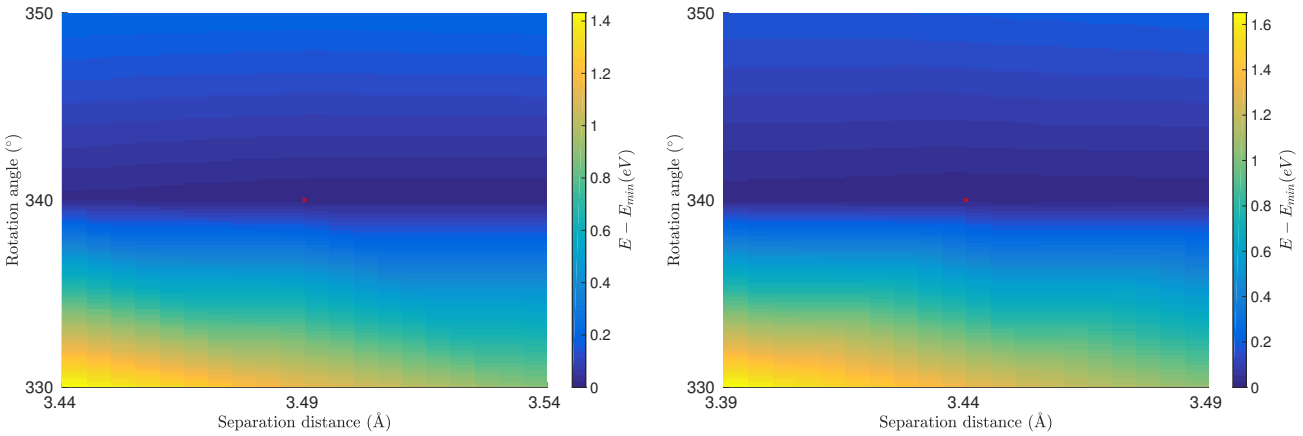
(d)


Rotation angle (°)
350
340
330
3.74
3.79
3.84
Separation distance (Å)
$E - E_{min}(eV)$
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9

(e)

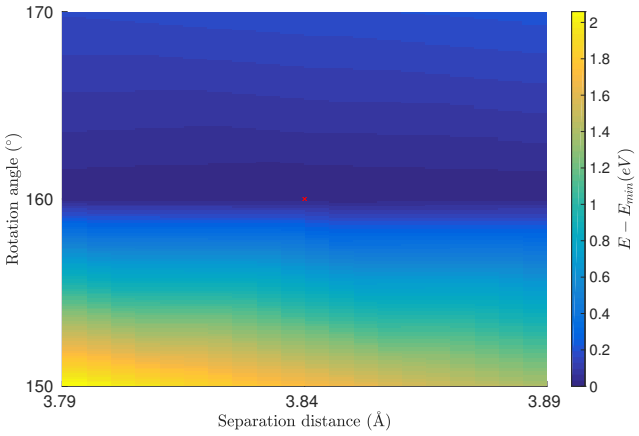

Rotation angle (°)
350
340
330
3.6
3.65
3.7
Separation distance (Å)
$E - E_{min}(eV)$
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9

(f)

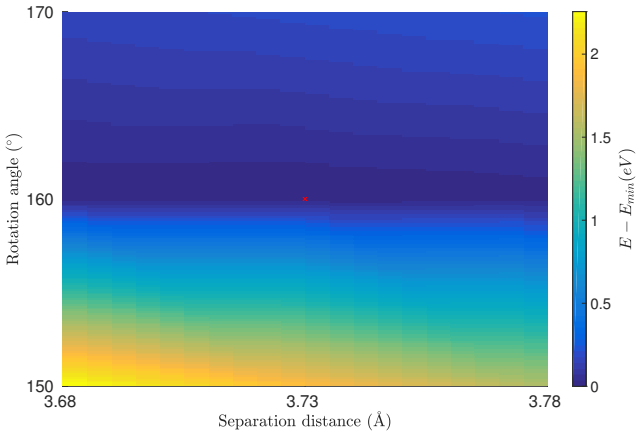


(g)

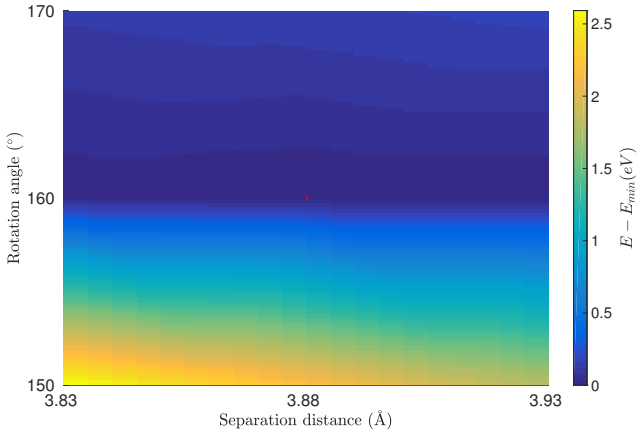
(h)



(i)

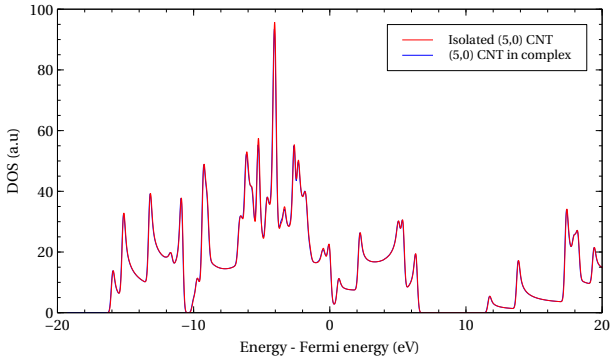


(j)

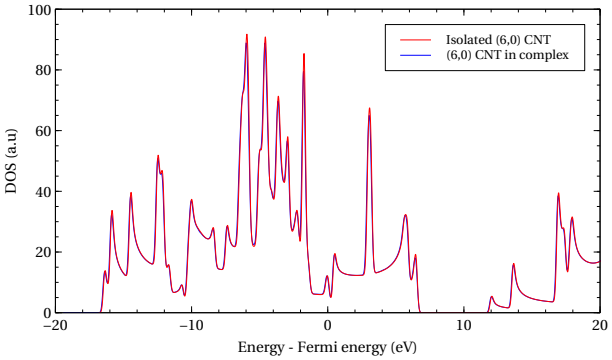


(k)

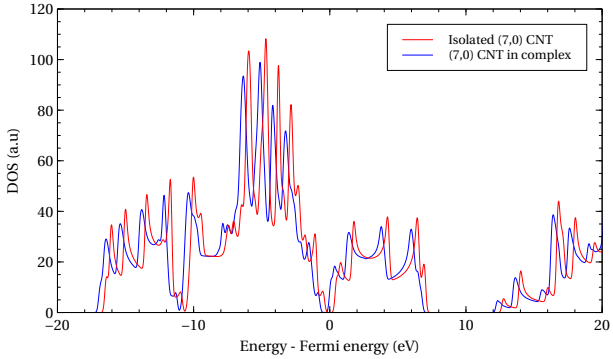
Figure S3: 2-D potential energy map for the complexes of the solvated AMP with : (a) (5,0) CNT, (b) (6,0) CNT, (c) (7,0) CNT, (d) (8,0) CNT, (e) (9,0) CNT, (f) (10,0) CNT, (g) (11,0) CNT, (h) (12,0) CNT, (i) (13,0) CNT, (j) (14,0) CNT, and (k) (15,0) CNT. The red colored × symbol represents the minimum energy.


Isolated (5,0) CNT
(5,0) CNT in complex
DOS (a.u)
Energy - Fermi energy (eV)

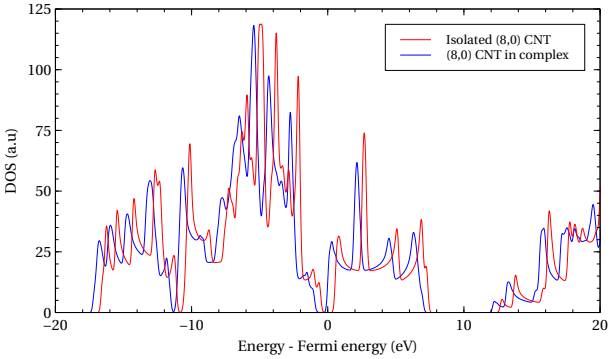
(a)


Isolated (6,0) CNT
(6,0) CNT in complex
DOS (a.u)
Energy - Fermi energy (eV)

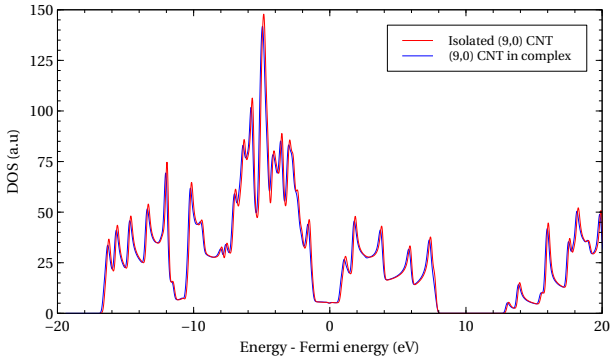
(b)


Isolated (7,0) CNT
(7,0) CNT in complex
DOS (a.u)
Energy - Fermi energy (eV)

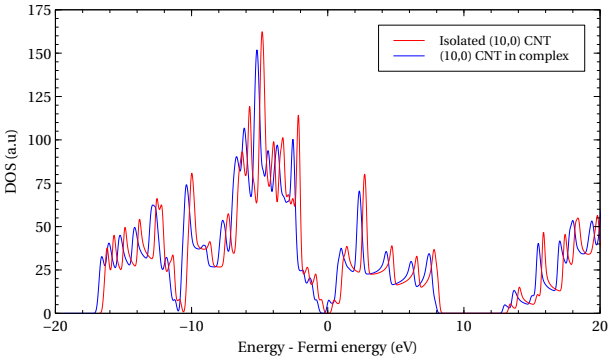
(c)


Isolated (8,0) CNT
(8,0) CNT in complex
DOS (a.u)
Energy - Fermi energy (eV)

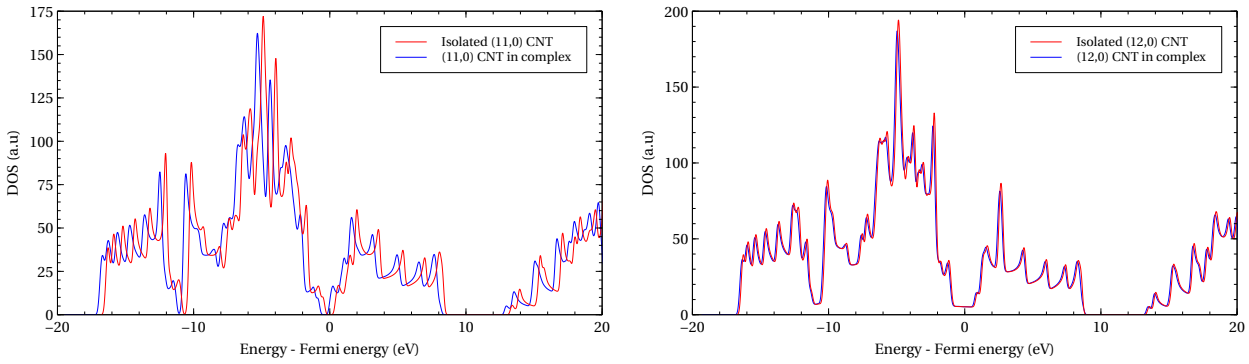
(d)


Isolated (9,0) CNT
(9,0) CNT in complex
DOS (a.u)
Energy - Fermi energy (eV)

(e)

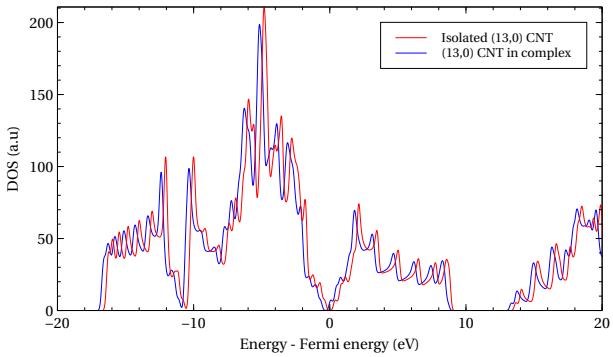

Isolated (10,0) CNT
(10,0) CNT in complex
DOS (a.u)
Energy - Fermi energy (eV)

(f)

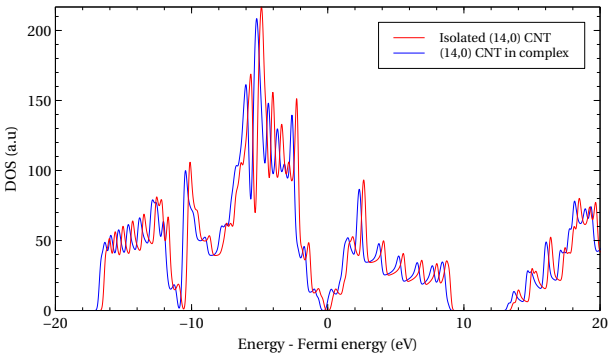


(g)

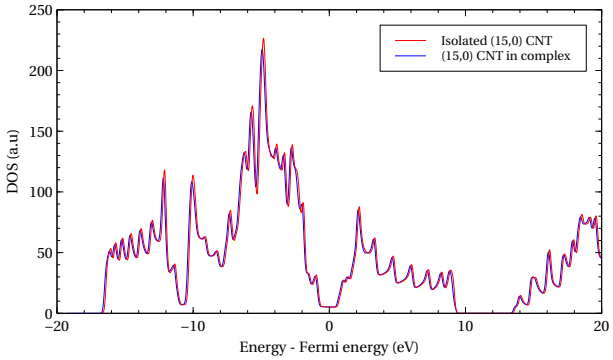
(h)



(i)



(j)



(k)

Figure S4: DOS for CNTs with the chirality of: (a) (5,0), (b) (6,0), (c) (7,0), (d) (8,0), (e) (9,0), (f) (10,0), (g) (11,0), (h) (12,0), (i) (13,0), (j) (14,0), and (k) (15,0). The red and blue colored curves respectively correspond to the isolated and the complexed CNT in vacuum

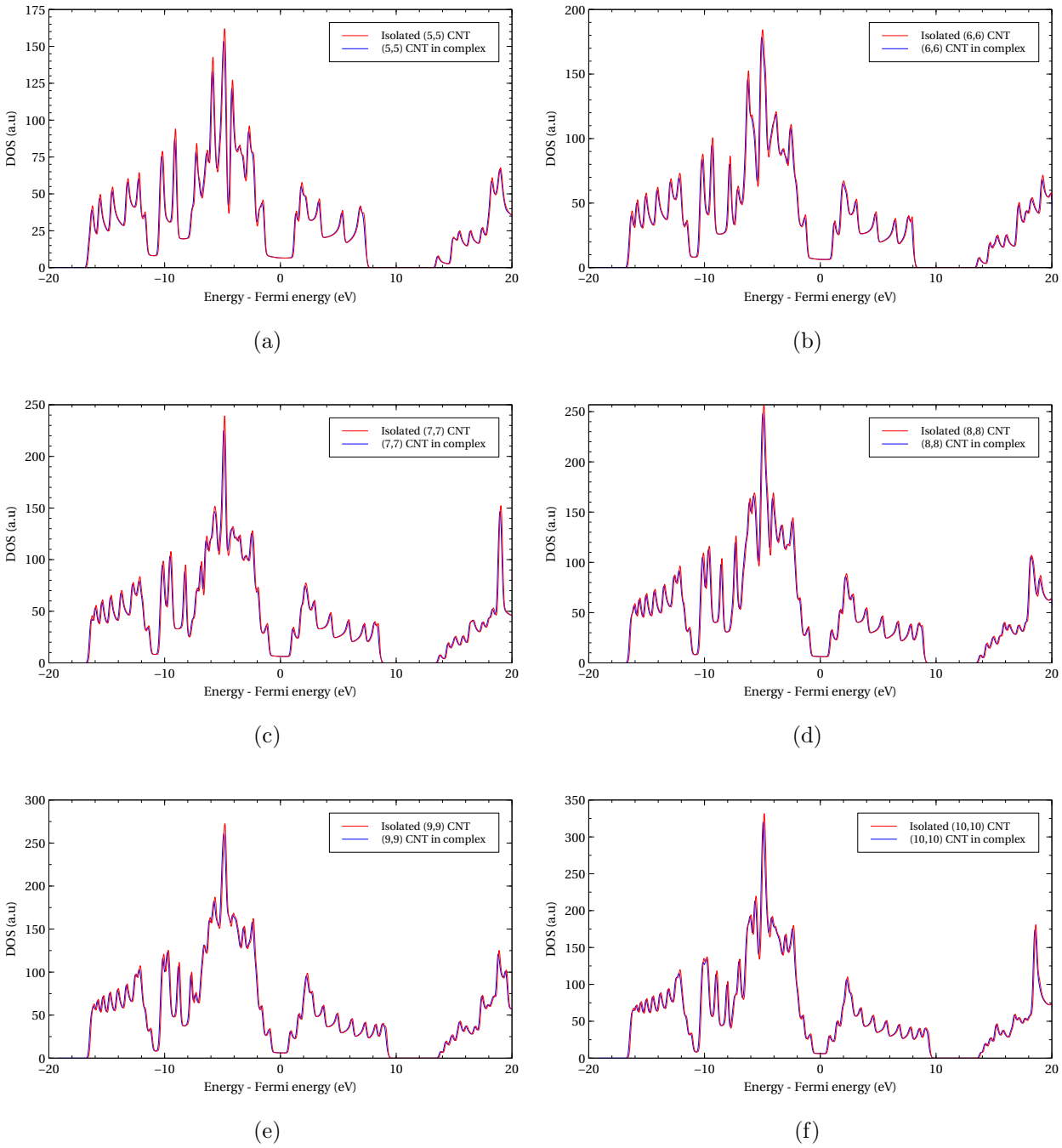
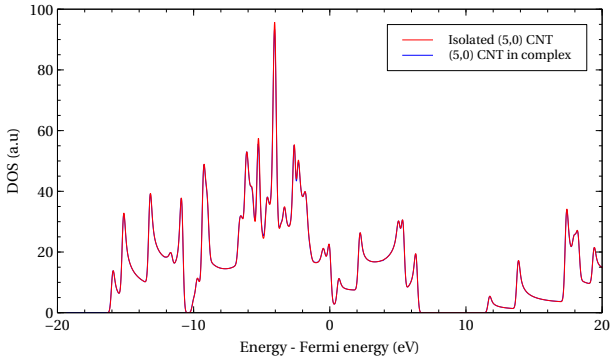
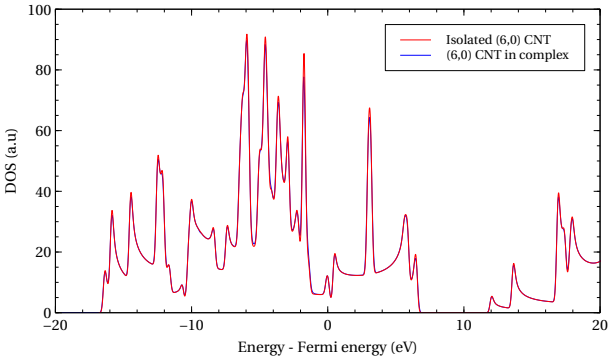


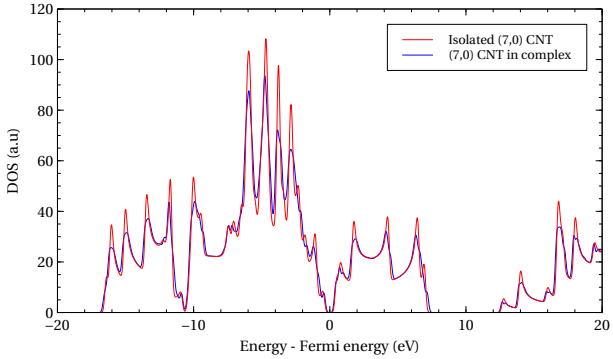
Figure S5: DOS for CNTs with the chirality of: (a) (5,5), (b) (6,6), (c) (7,7), (d) (8,8), (e) (9,9), and (f) (10,10). he red and blue colored curves respectively correspond to the isolated and the complexed CNT in vacuum.


Isolated (5,0) CNT
(5,0) CNT in complex
DOS (a.u)
Energy - Fermi energy (eV)

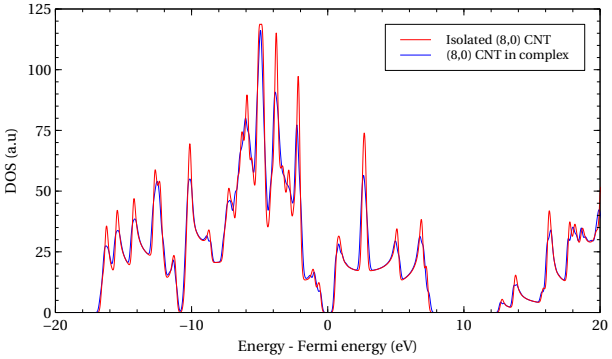
(a)


Isolated (6,0) CNT
(6,0) CNT in complex
DOS (a.u)
Energy - Fermi energy (eV)

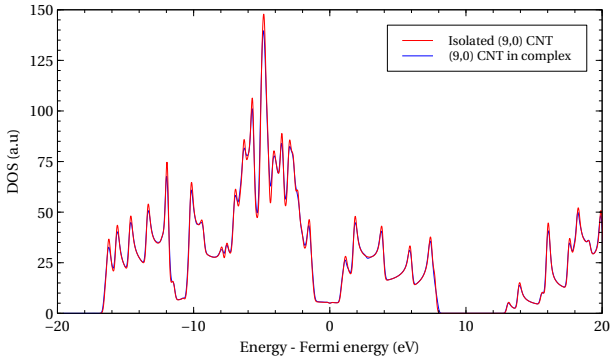
(b)


Isolated (7,0) CNT
(7,0) CNT in complex
DOS (a.u)
Energy - Fermi energy (eV)

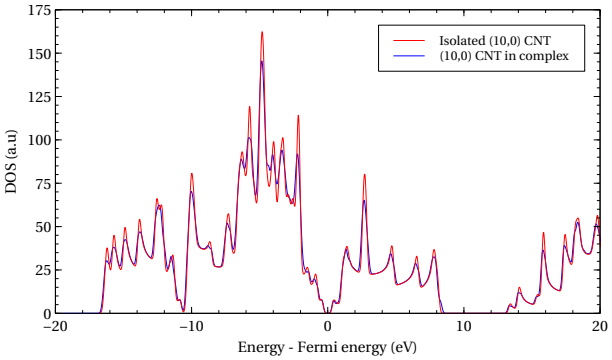
(c)


Isolated (8,0) CNT
(8,0) CNT in complex
DOS (a.u)
Energy - Fermi energy (eV)

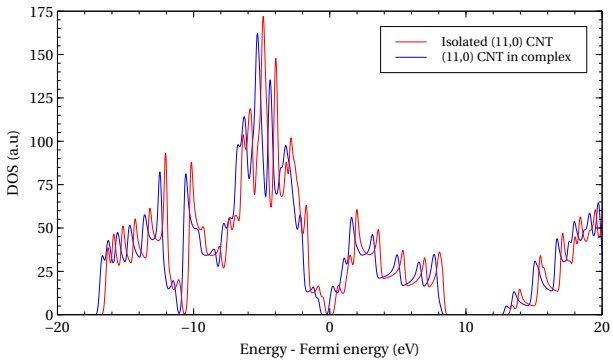
(d)


Isolated (9,0) CNT
(9,0) CNT in complex
DOS (a.u)
Energy - Fermi energy (eV)

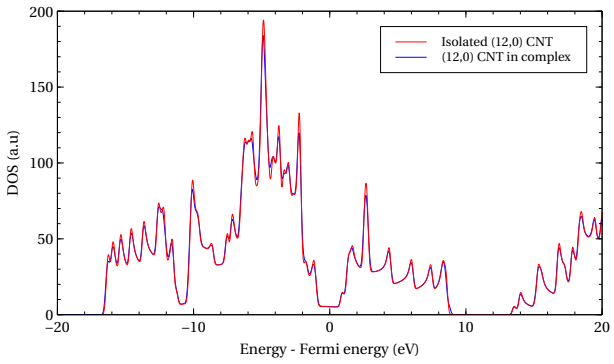
(e)


Isolated (10,0) CNT
(10,0) CNT in complex
DOS (a.u)
Energy - Fermi energy (eV)

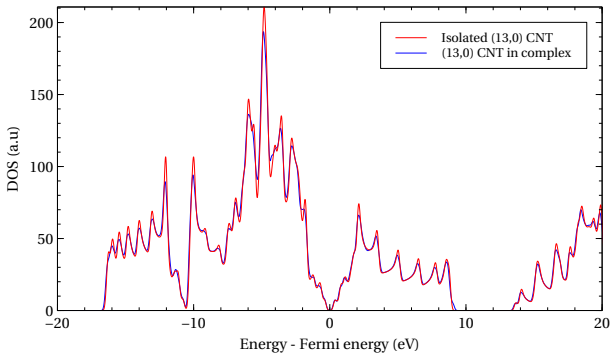
(f)



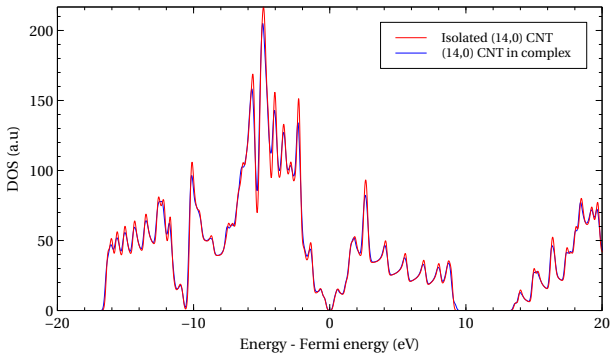
(g)



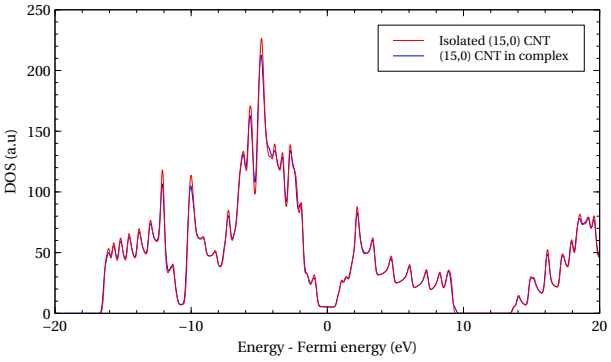
(h)



(i)



(j)



(k)

Figure S6: DOS for CNTs with the chirality of: (a) (5,0), (b) (6,0), (c) (7,0), (d) (8,0), (e) (9,0), (f) (10,0), (g) (11,0), (h) (12,0), (i) (13,0), (j) (14,0), and (k) (15,0). The red and blue colored curves respectively correspond to the isolated and the complexed CNT in solution.

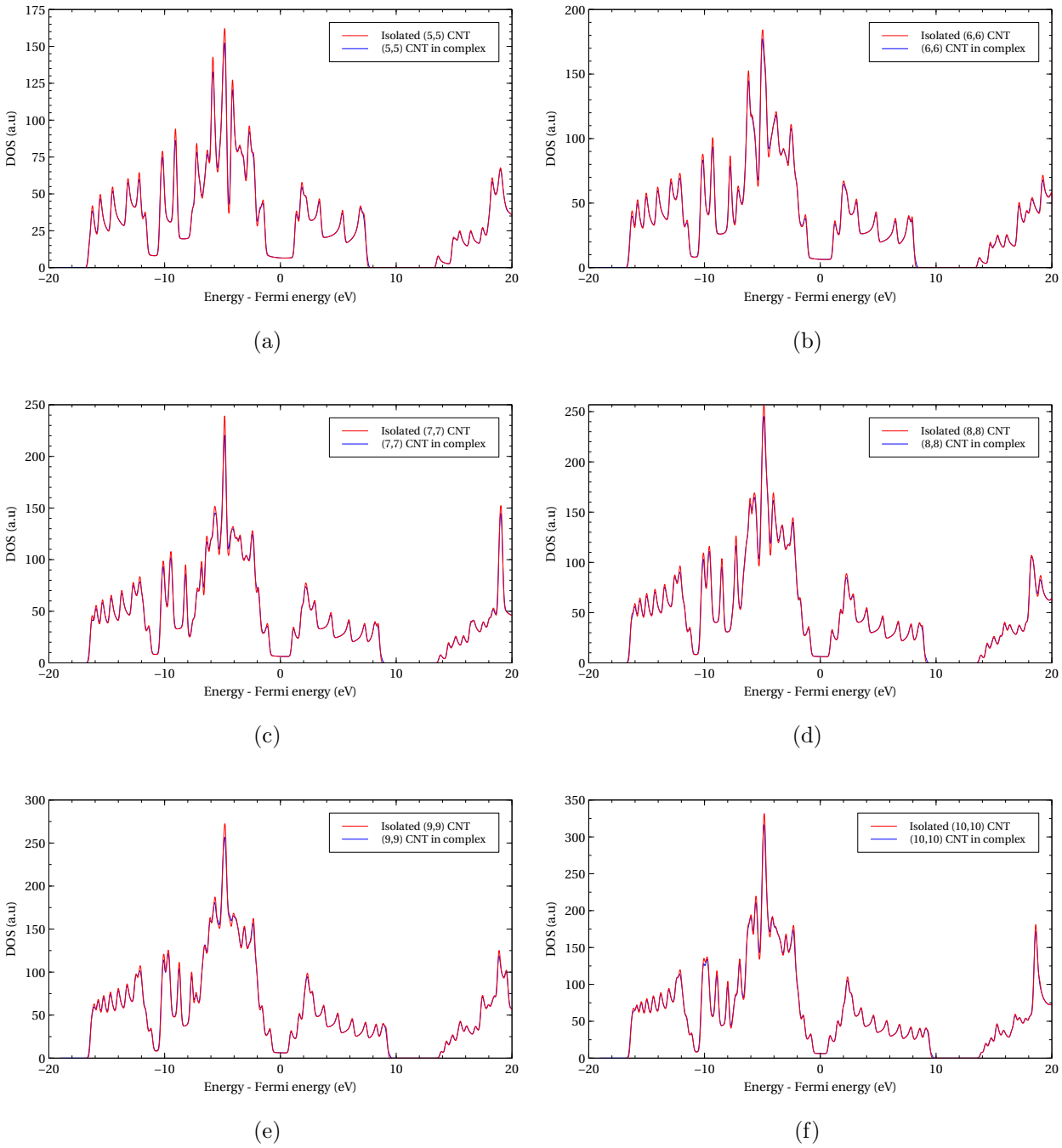


Figure S7: DOS for CNTs with the chirality of: (a) (5,5), (b) (6,6), (c) (7,7), (d) (8,8), (e) (9,9), and (f) (10,10). The red and blue colored curves respectively correspond to the isolated and the complexed CNT in solution.

References

(S1) Řezáč, J.; Riley, K. E.; Hobza, P. S66: A Well-balanced Database of Benchmark Interaction Energies Relevant to Biomolecular Structures. *Journal of Chemical Theory and Computation* **2011**, *7*, 2427–2438.