Supplementary material

March 27, 2015

This section contains additional information and tables about the geometry and the nature of the electronic states.

1 The table of geometry of nanotubes *n_p* (Å)

The section 1 presents the detailed geometry of the nanotubes. The D_{nd}/D_{nh} symmetry is respected and the symmetric atoms are assigned the same distance parameters.

The axis of the nanotube is taken as the z-axis, consequently, the distances of the atoms from the σ_h/σ_v plane are given by z_i. The radial distances from the axis of the nanotube are given r_i. The indices i distinguish symmetrically different atoms of the nanotube thus, all atoms which are equivalent in the symmetry group of the given nanotube have the same index i. Taking the hydrogen atoms for example, all the atoms have been assigned the same radial distance from the axis of the nanotube (rh) and the same longitudinal distance (zh) from the σ_h/σ_v plane of the nanotube. The rings of C atoms which makes up the body of the nanotube follow the same rule, the carbon atoms at the same distance z0, z1, .. above the σ_h plane for example, are at the same radial distance r0, r1, ... respectively from the axis of the nanotube.

Table 1: Nanotubes (n_p) where n=6 p=even

p	rh	r0	r1	r2	r3	r4	r5	r6
	zh	z0	z1	r2	z3	z4	z5	z6
2	2.38043	2.39593	2.39548	2.41332				
	3.55954	0.35020	1.79977	2.47664				
4	2.37984	2.40148	2.40054	2.39927	2.41438	2.39690		
	5.70045	0.35175	1.79061	2.49286	4.61762	3.94033		
6	2.38007	2.40445	2.40349	2.40326	2.39982	2.40114	2.39712	2.41464
	7.83959	0.35233	1.78782	2.49218	3.92973	4.63234	6.07937	6.75679

Table 2: Nanotubes (n_p) where n=6 p=odd

p	rh	r1	r2	r3	r4	r5	r6
	zh	z1	z2	z3	z4	z5	z6
1	2.37408	2.40928	2.39449				
	2.48737	0.72848	1.40452				
3	2.37975	2.39784	2.39939	2.39669	2.41409		
	4.63032	0.72046	1.42227	2.87034	3.54748		
5	2.37889	2.40301	2.40323	2.39951	2.39870	2.41418	2.39446
	6.77400	1.42870	0.71170	3.56871	2.85434	5.69110	5.00646

Table 3: Nanotubes (n_p) where n=7 p=even

p	rh	r0	r1	r2	r3	r4	r5	r6
	zh	z0	z1	z2	z3	z4	z5	z6
2	2.77780	2.78436	2.78531	2.80241				
	3.55398	0.35295	1.78992	2.47118				
4	2.77623	2.79032	2.78851	2.78818	2.80259	2.78640		
	5.68876	0.35450	1.78098	2.48864	4.60600	3.92447		
6	2.77645	2.79313	2.79167	2.79223	2.78882	2.78846	2.80272	2.78650
	7.82220	0.35491	1.77898	2.48857	4.62222	3.91433	6.05784	6.73944

Table 4: Nanotubes (n_p) where n=7 p=odd

p	rh	r1	r2	r3	r4	r5	r6
	zh	z1	z2	z3	z4	z5	z6
1	2.77417	2.80055	2.78521				
	2.48478	1.40199	0.72142				
3	2.77635	2.78667	2.78757	2.78633	2.80254		
	4.62170	0.71404	1.42138	2.85751	3.53893		
5	2.77754	2.79198	2.79131	2.78803	2.78841	2.78653	2.80331
	6.75554	0.71233	1.42172	2.84768	3.55557	4.99126	5.67273

Table 5: Nanotubes (n_p) where n=8 p=even

p	rh	r0	r1	r2	r3	r4	r5	r6
	zh	z0	z1	z2	z3	z4	z5	z6
2	3.15320	3.15577	3.15864	3.17467				
	3.56416	0.34999	1.80445	2.48143				
4	3.15298	3.16317	3.17687	3.16177	3.16230	3.16127		
	5.70706	0.35199	2.49564	1.79323	4.62437	3.94685		
6	3.14085	3.17056	3.16979	3.16972	3.16752	3.16781	3.14558	3.16399
	7.85805	0.35265	2.49270	1.78810	4.63263	3.93097	6.77092	6.08106

Table 6: Nanotubes (n_p) where n=8 p=odd

p	rh	r1	r2	r3	r4	r5	r6
	rh	r1	r2	r3	r4	r5	r6
1	3.14341	3.15724	3.16918				
	2.49010	0.73143	1.40740				
3	3.15302	3.15838	3.16014	3.16103	3.17627		
	4.63622	1.42395	0.72217	2.87625	3.55352		
5	3.15333	3.16571	3.16640	3.16330	3.16240	3.17737	3.16225
	6.77688	1.42362	0.71876	3.56602	2.86314	5.69419	5.01651

Table 7: Nanotubes (n_p) where n=9 p=even

p	rh zh	r0 z0	r1 z1	r2 z2	r3 z3	r4 z4	r5 z5	r6 z6
2	3.58513 3.54672	3.57454 0.35806	3.57769 1.77540	3.59746 2.46409				
4	3.54689 5.70286	3.55089 0.35280	3.55030 2.49352	3.54916 1.78972	3.56807 4.62018	3.55098 3.94270		
6	3.56757 7.91076	3.56989 0.34908	3.56705 2.48603	3.56827 1.78786	3.56343 4.62296	3.56303 3.78192	3.58407 6.76018	3.56477 6.06174

Table 8: Nanotubes (n_p) where n=9 p=odd

p	rh zh	r1 z1	r2 z2	r3 z3	r4 z4	r5 z5	r6 z6
1	3.54175 2.48727	3.56223 0.72861	3.55080 1.40453				
3	3.54943 4.62907	3.54914 0.71811	3.55073 1.42268	3.55312 2.86662	3.56716 3.54639		
5	3.54859 6.77060	3.55379 1.42288	3.55471 0.71655	3.55142 3.56229	3.55057 2.85804	3.56955 5.68789	3.55200 5.01014

2 State-specific energies

In this section, we report the state specific calculations for some representative of each class of nanotube. These calculations were carried out at the CAS-SCF level using the active space and the ROHF geometries described in the paper. The geometry was then optimized at the same level before inclusion of the dynamic correlation using the NEVPT2 method. The resulting state specific CASSCF (before and after geometry optimization) and NEVPT2 energies are reported in 9 and 10.

n_p	State	CAS-SCF	CAS-SCF	NEVPT2
			OPTIMIZED	
6_4	$^1A_1$	$2.44{\cdot}10^{-5}$	$2.63{\cdot}10^{-5}$	-5.89
	$^3A_2$	0.00	0.00	0.00
	^1E	250.74	249.00	276.79
6_5	$^1A_1$	$-3.13{\cdot}10^{-4}$	$-3.41{\cdot}10^{-4}$	-3.66
	$^3A_2$	0.00	0.00	0.00
	$^1E_2$	433.66	418.79	170.76

Table 9: State-specific energy differences for *e_p* nanotubes calculated by performing CAS-SCF separately for each state followed by geometry optimization and NEVPT2 calculation

n_p	State	CAS-SCF	CAS-SCF	NEVPT2
			OPTIMIZED	
7_4	$^1A_{1g}$	-0.98	-0.98	$-3.67{\cdot}10^{-3}$
	$^3A_{2u}$	-0.63	-0.63	$-2.43{\cdot}10^{-3}$
	$^5A_{1g}$	0.00	0.00	0.00
7_5	$^1A'_1$	-0.19	-0.19	-4.56
	$^3A"_2$	-0.13	-0.13	-3.06
	$^5A'_1$	0.00	0.00	0.00

Table 10: State-specific energy differences for *o_p* of nanotubes calculated by performing CAS-SCF separately for each state followed by geometry optimization and NEVPT2 calculation

3 The CI coefficients of the ground state wavefunction

The sections 3 and 4 give the CI vectors which result from the CAS-CI calculations for each of the four family of the nanotubes. It should be noted that in this part there are two/four orbitals for each nanotube and the configurations are made up of the two/four edge orbitals. The letter *a* represents the alpha spin and *b* the beta spin, double occupancy is marked by a *2* and empty orbitals by *0*. The orbitals for the *e_e* class of nanotubes consist of two degenerate e_3 orbitals where as the *e_o* class of nanotubes consist of two non-degenerate orbitals b_{1u} and b_{2g}. The four nanotubes for the *o_e* class of nanotubes consist of two pairs of degenerate orbitals e_{3g} and e_{3u} and similarly the *o_o* class of nanotubes two pairs of degenerate orbitals e_3' and e_3''. The electronic configuration can then be written for the *e_o* class of orbitals, for example, as follows, $0.707|b_{1u}\bar{b}_{1u} > +0.707|b_{2g}\bar{b}_{2g} >$.

Table 11: $^3A_2$ state CI vectors for 6_4 basis: STO-3G
the triplet coefficients are given in the m_s=0 subspace

configuration	coefficients
a b	0.707
b a	0.707

Table 12: $^3A_2$ state CI vectors for 6_4 basis: cc-pVDZ
the triplet coefficients are given in the m_s=0 subspace

configuration	coefficients
a b	0.707
b a	0.707

Table 13: ground state $^1A_{1g}$ CI vectors for 6_5 basis: STO-3G

configuration	coefficients
0 2	0.708
2 0	-0.707

Table 14: ground state $^1A_{1g}$ CI vectors for 6_5 basis: cc-pVDZ

configuration	coefficients
0 2	0.707
2 0	-0.706

Table 15: ground state $^1\mathrm{A}_{1g}$ CI vectors for 7_4 basis: STO-3G

configuration	coefficients
0 2 2 0	0.462
0 0 2 2	-0.432
2 2 0 0	-0.432
2 0 0 2	0.406
b a b a	-0.288
a b a b	-0.288
b b a a	0.144
a a b b	0.144
b a a b	0.144
a b b a	0.144

Table 16: ground state $^1A_{1g}$ CI vectors for 7_4 basis: cc-pVDZ

configuration	coefficients
0 2 2 0	0.443
2 2 0 0	-0.433
0 0 2 2	-0.433
2 0 0 2	0.423
b a b a	-0.289
a b a b	-0.289
a a b b	0.144
b b a a	0.144
b a a b	0.144
a b b a	0.144

Table 17: ground state $^1A_1'$ CI vectors for 7_5 basis: STO-3G

configuration	coefficients
0 0 2 2	0.445
2 0 0 2	-0.433
0 2 2 0	-0.433
2 2 0 0	0.421
b a b a	0.288
a b a b	0.288
b a a b	-0.144
a b b a	-0.144
b b a a	-0.144
a a b b	-0.144

Table 18: ground state $^1A_1'$ CI vectors for 7_5 basis: cc-pVDZ

configuration	coefficients
0 0 2 2	0.437
2 0 0 2	-0.433
0 2 2 0	-0.433
2 2 0 0	0.429
b a b a	0.289
a b a b	0.289
b a a b	-0.144
a b b a	-0.144
b b a a	-0.144
a a b b	-0.144

4 The CI coefficients of the excited state wavefunctions

Table 19: ground state $^1A_1$ CI vectors for 6_4 basis: STO-3G

configuration	coefficients
a b	-0.707
b a	0.707

Table 20: ground state $^1A_1$ CI vectors for 6_4 basis: cc-pVDZ

configuration	coefficients
a b	-0.707
b a	0.707

Table 21: $^1E_2$ state CI vectors for 6_4 basis: STO-3G

configuration	coefficients
0 2	-0.707
2 0	0.707

Table 22: $^1E_2$ state CI vectors for 6_4 basis: cc-pVDZ

configuration	coefficients
0 2	-0.707
2 0	0.707

Table 23: $^3A_{2u}$ state ci vectors for 6_5 basis: STO-3G

configuration	coefficients
a a	1.000

Table 24: $^3A_{2u}$ state ci vectors for 6_5 basis: cc-pVDZ

configuration	coefficients
a a	1.000

Table 25: $^1E_{1g}$ state ci vectors for 6_5 basis: STO-3G

configuration	coefficients
a b	0.708
b a	-0.707

Table 26: $^1E_{1g}$ state ci vectors for 6_5 basis: cc-pVDZ

configuration	coefficients
a b	0.707
b a	-0.707

Table 27: $^3A_{2u}$ state ci vectors for 7_4 basis: STO-3G

configuration	coefficients
0 a 2 a	-0.516
a 2 a 0	0.516
a 0 a 2	-0.484
2 a 0 a	0.484

Table 28: $^5A_{1g}$ state ci vectors for 7_4 basis: STO-3G

configuration	coefficients
a a a a	1.000

Table 29: $^3A_{2u}$ state ci vectors for 7_4 basis: cc-pVDZ

configuration	coefficients
a 2 a 0	0.506
0 a 2 a	-0.506
2 a 0 a	0.494
a 0 a 2	-0.494

Table 30: $^5A_{1g}$ state ci vectors for 7_4 basis: cc-pVDZ

configuration	coefficients
a a a a	1.000

Table 31: $^3A_2^{''}$ state ci vectors for 7_5 basis: STO-3G

configuration	coefficients
a 0 a 2	0.507
0 a 2 a	0.507
2 a 0 a	-0.493
a 2 a 0	-0.493

Table 32: $^5A_1^{'}$ state ci vectors for 7_5 basis: STO-3G

configuration	coefficients
a a a a	1.000

Table 33: $^3A_2^{''}$ state ci vectors for 7_5 basis: cc-pVDZ

configuration	coefficients
a 0 a 2	0.502
0 a 2 a	0.502
2 a 0 a	-0.498
a 2 a 0	-0.498

Table 34: $^5A_1^{'}$ state ci vectors for 7_5 basis: cc-pVDZ

configuration	coefficients
a a a a	1.000