

Supporting Information

Theoretical Studies on Structures, ^{13}C NMR Chemical Shifts, Aromaticity, and Chemical Reactivity of Finite-Length Open-Ended Armchair Single-Walled Carbon Nanotubes

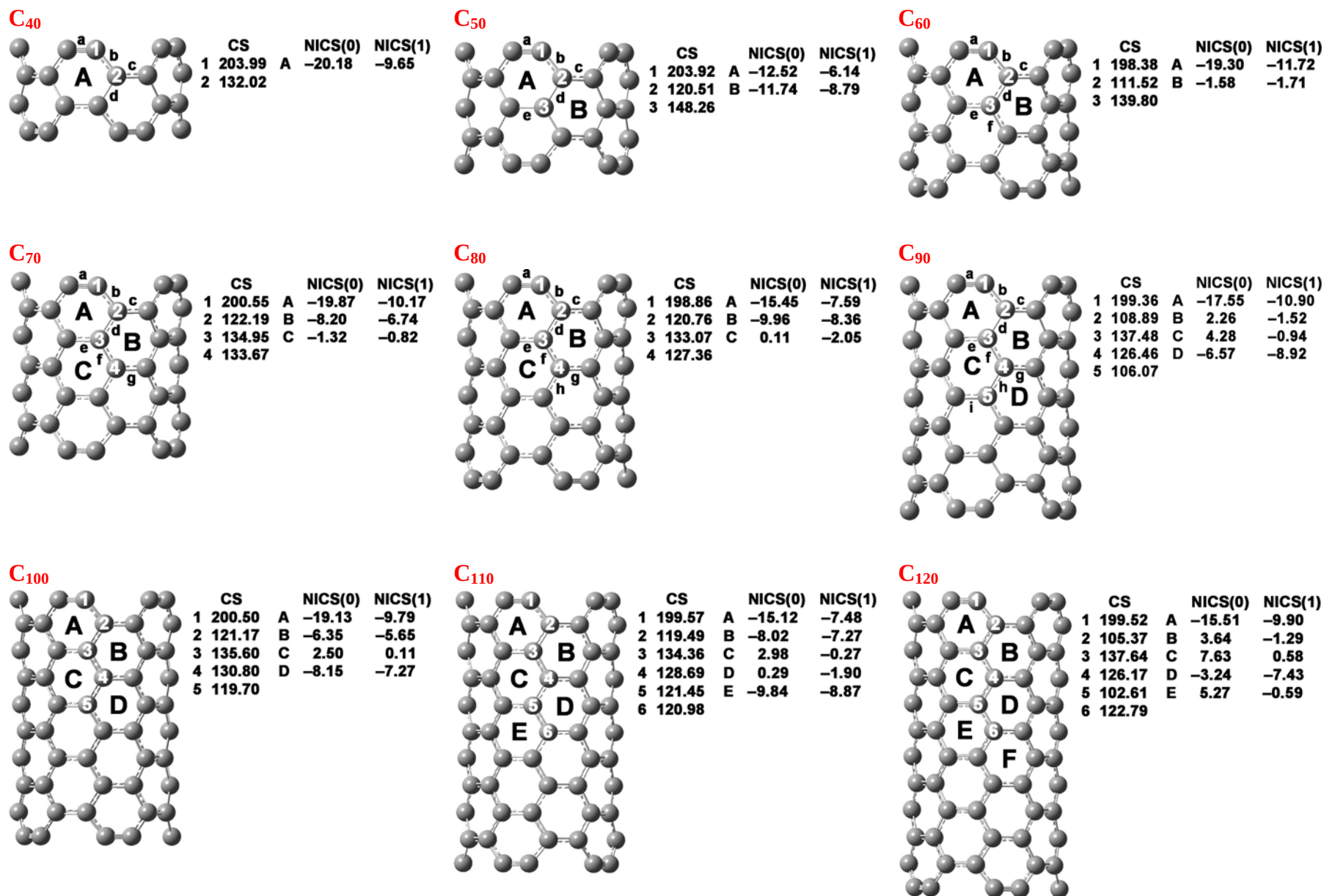
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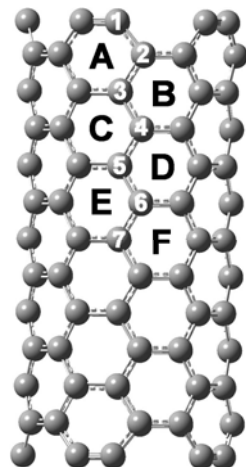
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Changchun, Jilin 130023, China*

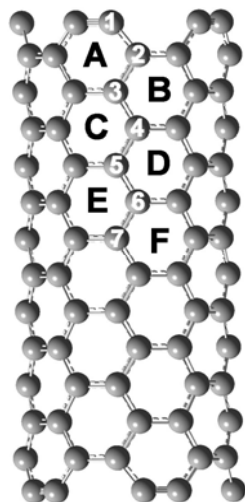
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Figure S1. ^{13}C NMR chemical shifts (CS) and nucleus independent chemical shifts (NICS) of the finite-length open-ended (5,5) SWCNTs C_{40} – C_{180} .

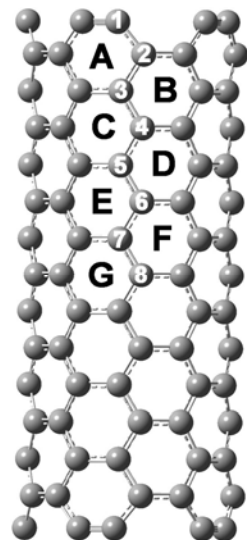


C₁₃₀

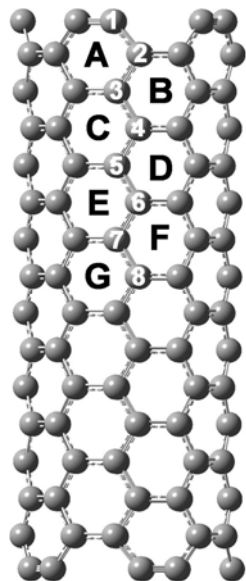
	CS		NICS(0)	NICS(1)
1	200.68	A	-17.86	-9.31
2	118.57	B	-4.86	-4.91
3	136.04	C	4.22	0.84
4	130.50	D	-6.31	-6.50
5	118.20	E	-5.98	-6.13
6	120.40	F	4.13	1.21
7	127.26			

C₁₄₀

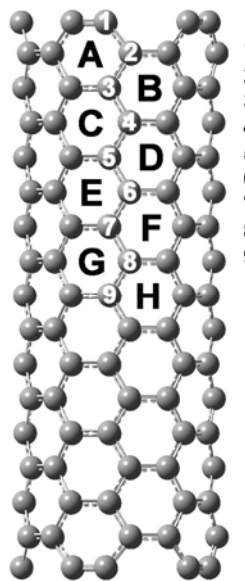
	CS		NICS(0)	NICS(1)
1	200.01	A	-14.81	-7.40
2	118.26	B	-6.38	-6.38
3	135.58	C	4.68	0.64
4	129.41	D	0.66	-2.02
5	119.87	E	-7.99	-7.96
6	121.60	F	3.66	0.10
7	122.96			

C₁₅₀

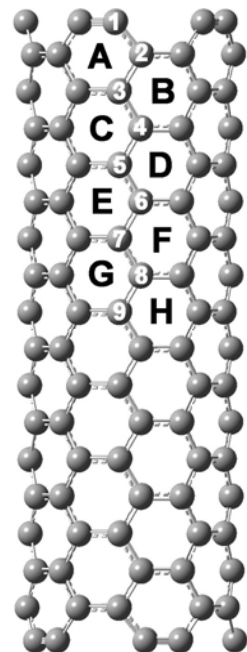
	CS		NICS(0)	NICS(1)
1	199.72	A	-13.44	-8.98
2	102.37	B	5.22	-0.89
3	138.03	C	10.70	1.89
4	125.18	D	0.32	-5.89
5	98.77	E	7.26	-0.30
6	122.29	F	9.72	1.19
7	121.09	G	1.02	-5.77
8	98.07			

C₁₆₀

	CS		NICS(0)	NICS(1)
1	200.84	A	-16.72	-8.80
2	116.58	B	-3.24	-4.30
3	136.54	C	4.51	1.32
4	130.17	D	-4.36	-5.70
5	115.83	E	-3.96	-5.26
6	120.54	F	6.13	2.00
7	126.73	G	3.71	-5.24
8	118.58			

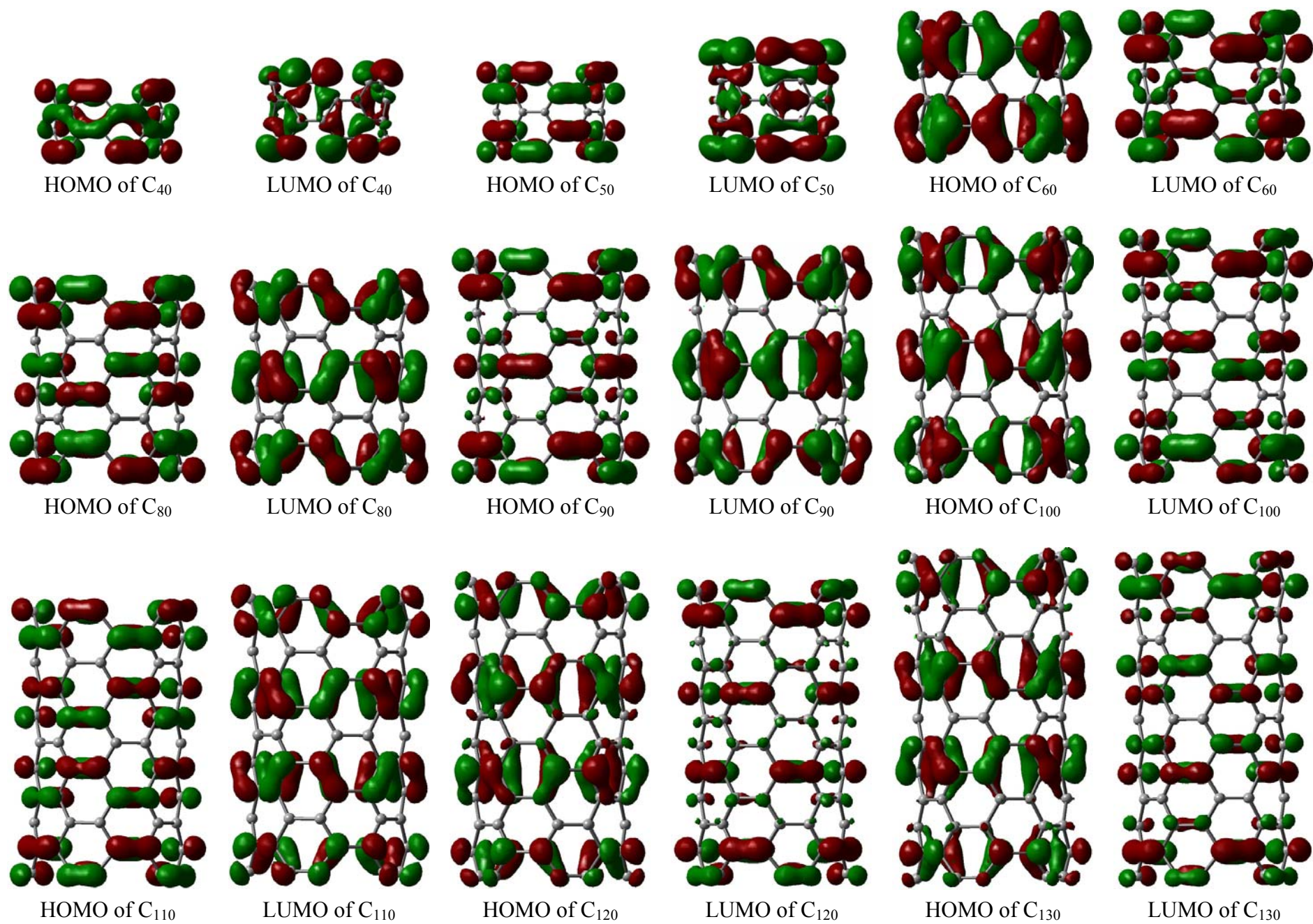
C₁₇₀

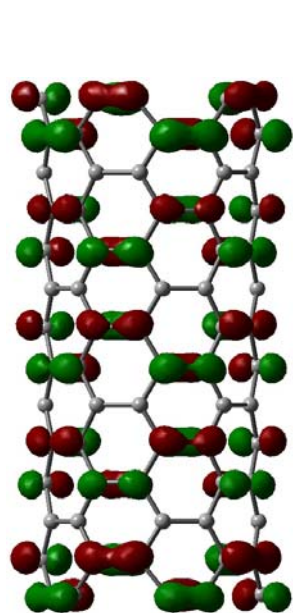
	CS		NICS(0)	NICS(1)
1	200.37	A	-14.59	-7.36
2	117.28	B	-5.12	-5.69
3	136.01	C	5.80	1.21
4	129.75	D	0.91	-2.12
5	118.37	E	-6.29	-7.11
6	121.31	F	5.82	1.22
7	123.80	G	4.28	0.09
8	121.35	H	-6.11	-7.17
9	121.36			

C₁₈₀

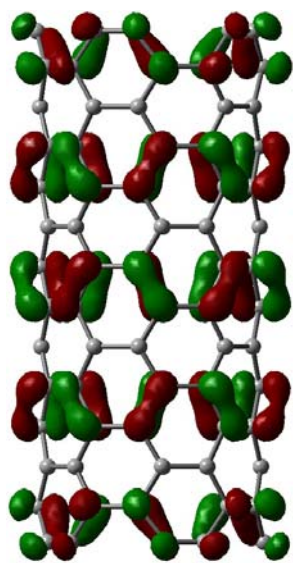
	CS		NICS(0)	NICS(1)
1	199.81	A	-11.51	-7.84
2	99.61	B	6.84	-0.48
3	138.51	C	13.49	2.50
4	124.42	D	3.83	-4.50
5	95.57	E	9.53	0.22
6	122.09	F	13.96	2.15
7	118.82	G	5.61	-4.14
8	93.21	H	12.76	1.97
9	119.86			

Figure S2. The HOMOs and the LUMOs of open-ended SWCNTs C_{40} – C_{180} .

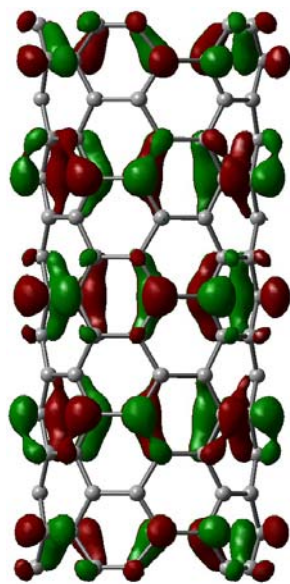




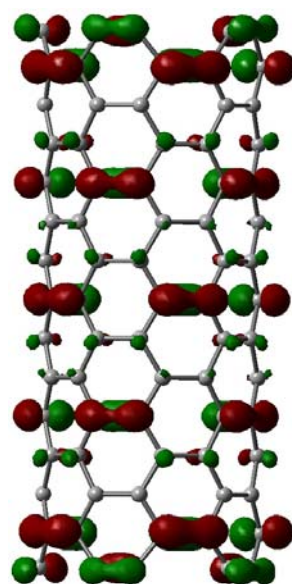
HOMO of C_{140}



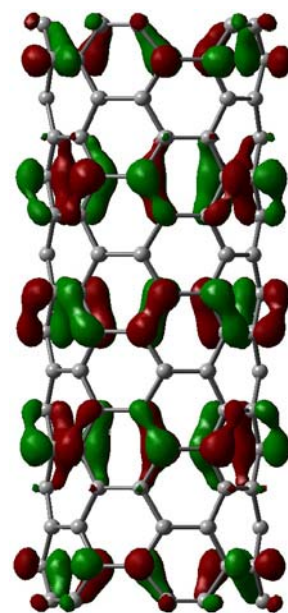
LUMO of C_{140}



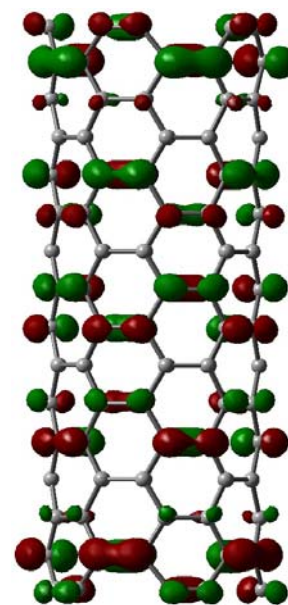
HOMO of C_{150}



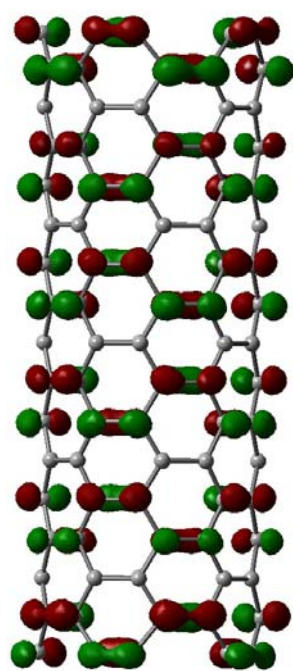
LUMO of C_{150}



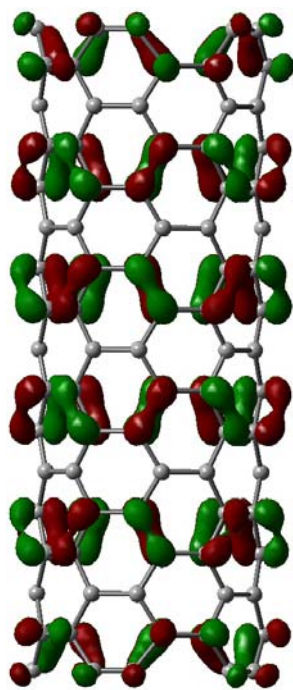
HOMO of C_{160}



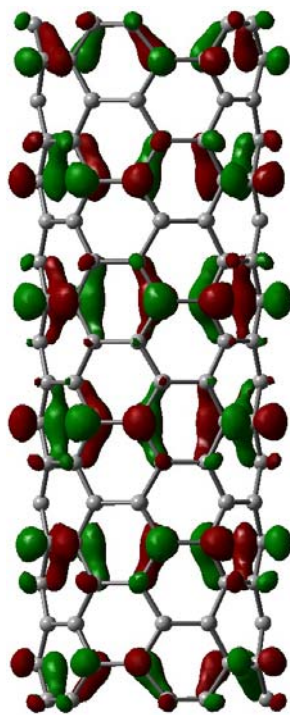
LUMO of C_{160}



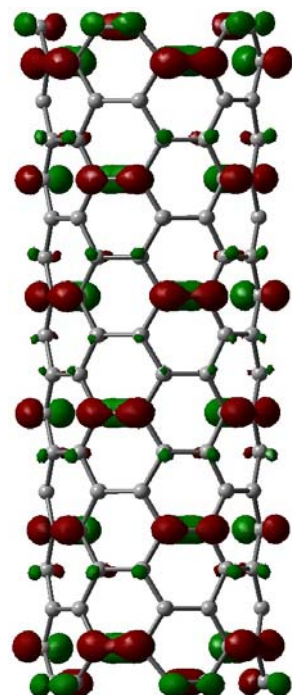
HOMO of C_{170}



LUMO of C_{170}



HOMO of C_{180}



LUMO of C_{180}