Supplemental Information

for

The Origin of Linear Relationship between CH_2/NH/O-SWNT Reaction Energies and Sidewall Curvature: Armchair Nanotubes

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Table S1. The 1/*d* value (in $Å^{-1}$, with positive and negative values for exo and endohedral interactions) and the reaction energy ΔE and their EDA components (in kcal/mol, see text for individual terms) at HF/STO-3G level for the reaction of CH_2 on (n,n) armchair SWNT.

Table S2. Relevant Fock and overlap matrix elements and diagonalized eigenvalues in the fragment MO basis set for a_1 SWNT→CH_2 donation and b_1 CH_2→SWNT backdonation processes in case of 5 Å 2-layer model compounds at the RHF/STO-3G level of theory for endo CH_2-(4,4) SWNT and exo(*s*) CH_2-(8,8) SWNT.

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Table S1. The 1/*d* value (in $Å^{-1}$, with positive and negative values for exo and endohedral interactions) and the reaction energy ΔE and their EDA components (in kcal/mol, see text for individual terms) at HF/STO-3G level for the reaction of CH_2 on (n,n) armchair SWNT.

	Endo										Exo(s)					
	n=4	5	6	7	8	9	10	11	12	13	n=13	12	11	10	9	8
1/*d*	-0.1796	-0.1446	-0.1210	-0.1039	-0.0911	-0.0810	-0.0730	-0.0664	-0.0609	-0.0562	0.0562	0.0609	0.0664	0.0730	0.0810	0.0911
DEF(SWCNT)	62.0	53.5	41.9	45.6	43.4	43.5	41.1	40.3	40.7	40.1	42.3	42.6	42.6	42.8	45.0	45.2
DEF(CH_2)	47.3	46.6	47.2	46.1	46.1	46.0	46.0	45.9	45.9	46.0	47.2	47.3	47.4	47.5	47.7	48.0
INT	-142.0	-150.7	-153.5	-155.8	-157.9	-159.6	-161.3	-162.9	-164.3	-165.7	-199.8	-201.4	-203.2	-205.6	-206.3	-215.0
ES	-117.5	-114.4	-114.0	-114.7	-115.0	-115.6	-116.3	-116.9	-117.5	-118.1	-140.1	-141.4	-142.7	-144.3	-147.3	-151.4
EX	308.6	296.3	294.4	294.4	293.9	294.2	294.5	294.7	295.0	295.2	318.3	319.7	321.1	322.9	326.3	331.2
ORB	-333.0	-332.6	-333.8	-335.5	-336.8	-338.1	-339.5	-340.7	-341.8	-342.9	-377.9	-379.8	-381.7	-384.1	-388.5	-394.8

Table S2.

Relevant Fock and overlap matrix elements and diagonalized eigenvalues in the fragment MO basis set for a_1 SWCNT→CH_2 donation and b_1 CH_2→SWCNT backdonation processes in case of 5 Å 2-layer model compounds at the RHF/STO-3G level of theory for endo CH_2-(4,4) SWNT and exo(*s*) CH_2-(8,8) SWNT. Energy units are [ha].

endo CH2-(4,4) SWCNT

Fock matrix			Overlap matrix			eigenvalues
			b1 backdonation			
CH2 HOMO	CNT π*		CH2 HOMO	CNT π*		
-0.223546			1.000000			-0.248653
0.130813	0.183801		-0.107026	1.000000		0.236773
			a1 donation			
CH2 LUMO	CNT π	CNT π	CH2 LUMO	CNT π	CNT π	
-0.497616			1.000000			-0.567078
-0.251960	-0.280359		-0.220492	1.000000		-0.130320
-0.108687	-0.017053	-0.275073	-0.095369	0.000000	1.000000	-0.264093

exo (CH2)-(8,8) SWCNT

Fock matrix			Overlap matrix			eigenvalues
			b1 backdonation			
CH2 HOMO	CNT π*		CH2 HOMO	CNT π*		
-0.265653			1.000000			-0.350291
0.272295	0.064229		-0.242620	1.000000		0.276661
			a1 donation			
CH2 LUMO	CNT π	CNT π	CH2 LUMO	CNT π	CNT π	
-0.552495			1.000000			-0.583182
-0.179086	-0.287318		-0.159841	1.000000		-0.211427
-0.082506	-0.020946	-0.228496	-0.074528	0.000000	1.000000	-0.229057