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APPENDICES

Table A1 Energy gaps of platinum atom and cluster adsorbed on various sizes of closed-end SWCNTs.

Reaction	E_{HOMO} [a]	E_{LUMO} [a]	E_g [a]	η [b]	μ [c]	χ [d]	ω [e]	DM [f]
Pt adatom:								
Clean	-5.44	-2.93	2.52	1.26	-4.18	1.26	6.95	0.00
Pt(1)/(3,3)_SWCNT	-5.43	-3.12	2.31	1.16	-4.28	1.16	7.91	0.26
Pt(2)/(3,3)_SWCNT	-5.41	-3.68	1.73	0.86	-4.54	0.86	11.94	0.68
Pt(3)/(3,3)_SWCNT	-5.40	-3.56	1.84	0.92	-4.48	0.92	10.92	0.45
Pt(4)/(3,3)_SWCNT	-5.25	-3.47	1.79	0.89	-4.36	0.89	10.65	0.44
Pt(5)/(3,3)_SWCNT	-5.25	-3.52	2.35	0.87	-4.38	0.87	11.09	0.14
Pt(6)/(3,3)_SWCNT	-5.55	-3.20	1.73	1.18	-4.38	1.18	8.15	0.62
Pt(7)/(3,3)_SWCNT	-5.37	-3.24	2.14	1.07	-4.30	1.07	8.68	0.30
Pt(8)/(3,3)_SWCNT	-5.33	-3.47	1.86	0.93	-4.40	0.93	10.42	0.51
Clean	-5.32	-4.04	1.28	0.64	-4.68	0.64	17.07	0.00
Pt(1)/(4,4)_SWCNT	-5.35	-4.06	1.29	0.64	-4.70	0.64	17.19	0.64
Pt(2)/(4,4)_SWCNT	-5.33	-4.08	1.25	0.62	-4.70	0.62	17.70	0.26
Pt(3)/(4,4)_SWCNT	-5.26	-4.27	1.33	0.50	-4.77	0.50	22.76	0.37
Pt(4)/(4,4)_SWCNT	-5.25	-3.95	1.00	0.65	-4.60	0.65	16.26	0.60
Pt(5)/(4,4)_SWCNT	-5.26	-4.10	1.30	0.58	-4.68	0.58	18.95	0.59
Pt(6)/(4,4)_SWCNT	-5.26	-4.02	1.16	0.62	-4.64	0.62	17.37	0.48
Pt(7)/(4,4)_SWCNT	-5.38	-4.03	1.24	1.26	-4.18	1.26	16.39	0.19
Clean	-4.79	-3.75	1.03	0.52	-4.27	0.52	17.64	0.00
Pt(1)/(5,5)_SWCNT	-4.82	-3.75	1.07	0.54	-4.29	0.54	17.09	0.41
Pt(2)/(5,5)_SWCNT	-4.75	-3.73	1.02	0.51	-4.24	0.51	17.56	0.88
Pt(3)/(5,5)_SWCNT	-4.81	-3.77	1.04	0.52	-4.29	0.52	17.78	0.45
Pt(4)/(5,5)_SWCNT	-4.78	-3.69	1.09	0.55	-4.24	0.55	16.46	0.91
Pt(5)/(5,5)_SWCNT	-4.74	-3.92	0.82	0.41	-4.33	0.41	22.92	0.79
Pt(6)/(5,5)_SWCNT	-4.88	-3.69	1.19	0.60	-4.29	0.60	15.43	0.43
Pt(7)/(5,5)_SWCNT	-4.86	-3.68	1.18	0.59	-4.27	0.59	15.43	0.23
Pt clusters:								
Pt_2/(3,3)_SWCNT	-5.40	-3.14	2.26	1.13	-4.27	1.13	8.09	0.73
Pt_3/(3,3)_SWCNT	-5.35	-3.26	2.09	1.05	-4.31	1.05	8.86	1.14
Pt_4/(3,3)_SWCNT	-5.11	-4.11	1.00	0.50	-4.61	0.50	21.28	1.12
Pt_2/(4,4)_SWCNT	-5.01	-3.92	1.09	0.54	-4.47	0.54	18.34	0.88
Pt_3/(4,4)_SWCNT	-4.92	-3.96	0.95	0.48	-4.44	0.48	20.70	1.23
Pt_4/(4,4)_SWCNT	-5.19	-4.24	0.95	0.48	-4.71	0.48	23.34	2.00
Pt_2/(5,5)_SWCNT	-4.81	-3.75	1.06	0.53	-4.28	0.53	17.31	0.29
Pt_3/(5,5)_SWCNT	-4.78	-3.74	1.03	0.52	-4.26	0.52	17.59	0.79
Pt_4/(5,5)_SWCNT	-4.88	-4.18	0.70	0.35	-4.53	0.35	29.28	4.50

[a] In eV.

[b] Chemical hardness, $\eta = E_g / 2$

[c] Electronic chemical potential, $\mu = (E_{HOMO} - E_{LUMO})/2$

[d] The Mulliken electronegativity index, $\chi = (-E_{HOMO} - E_{LUMO})/2$

[e] The electrophilicity index, $\omega = \mu^2 / 2\eta$, [f] Dipole moment, in Debye.

Table A2 Adsorption energies (ΔE_{ads}) of H_2 on platinum clusters, computed at the B3LYP/GEN[a] level of theory.

Hydrogen adsorption	ΔE_{ads} [b]
Pt-clusters :	
H_2/Pt_2	-56.75
H_2/Pt_3	-20.50
H_2/Pt_4 (square planar)	-20.54
H_2/Pt_4 (tetrahedral)	-26.03
H_2/Pt_5 (planar)	-29.67
H_2/Pt_5 (square pyramid)	-29.65
H_2/Pt_5 (trigonal bipyramid)	-29.70

[a] LanL2DZ for Pt atoms and 6-311++G(d,p) for hydrogen atoms.

[b] In kcal/mol.

Table A3 Geometrical parameters for free platinum clusters (Pt_4) and Pt_4 decorated on caps of (3,3), (4,4) and (5,5) SWCNTs.

Parameters[a]	Pt_4 clusters			
	Free[b]	(3,3)[c]	(4,4)[c]	(5,5)[c]
Bond length (Å):				
Pt1-Pt2	2.690	3.593	3.284	3.114
Pt2-Pt3	2.690	3.596	3.368	3.116
Pt2-Pt3	2.710	3.696	3.881	3.090
Pt1-Pt4	2.690	2.726	2.547	2.682
Pt2-Pt4	2.690	2.730	2.705	2.624
Pt3-Pt4	2.690	2.717	2.543	2.681
Bond angle (°):				
Pt1-Pt2-Pt3	60.5	60.0	71.4	59.5
Pt2-Pt3-Pt1	59.7	59.9	53.3	60.2
Pt3-Pt1-Pt2	59.7	60.0	55.3	60.3
Pt1-Pt4-Pt2	62.4	82.4	77.3	71.9
Pt2-Pt4-Pt3	62.4	82.6	79.8	71.9
Pt3-Pt4-Pt1	60.5	82.7	99.4	70.1

[a] Atomic labeling for platinum atoms is defined in Figure A3.

[b] Tetrahedral structure. ,[c] Distort tetrahedral structure.

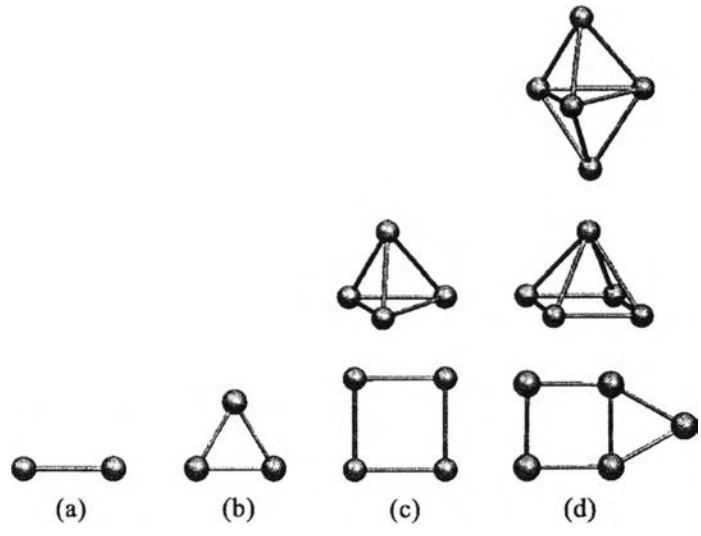

Figure A1. The B3LYP/LanL2DZ-optimized structures of Pt clusters (a) Pt_2, (b) Pt_3, (c) Pt_4, and (d) Pt_5.

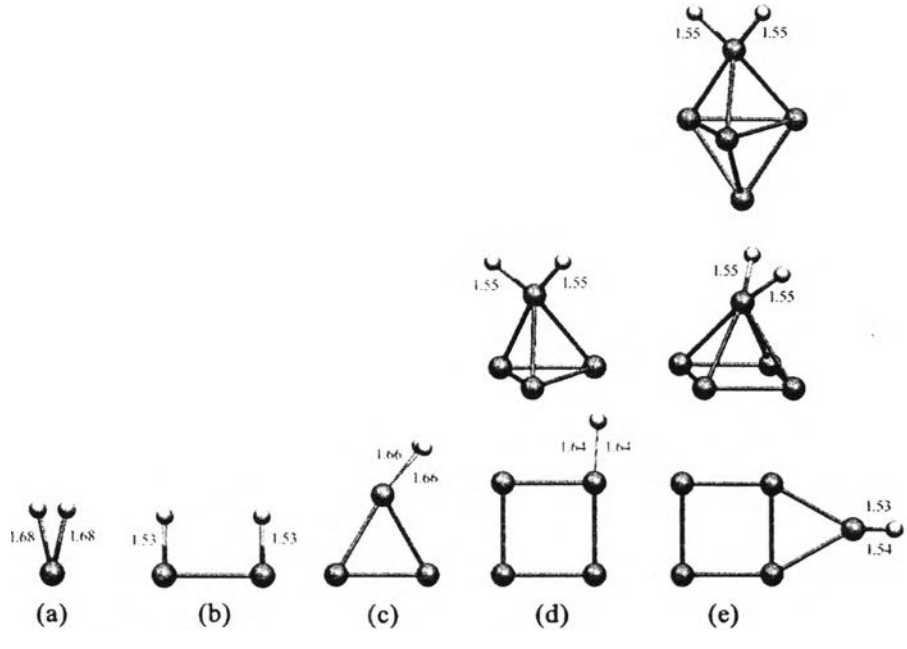

Figure A2. The B3LYP/GEN-optimized structures of hydrogen molecule adsorbed on (a) Pt atom, (b) Pt_2, (c) Pt_3, (d) Pt_4, and (e) Pt_5 clusters. B3LYP/GEN, GEN basis sets are as LanL2DZ for Pt atoms and 6-311++G(d,p) for hydrogen atoms. Their bond distances are in Å.

Figure A3. The B3LYP/LanL2DZ–optimized structures of (a) free tetra platinum cluster (Pt_4) and Pt_4 decorated on caps of (b) (3,3), (c) (4,4) and (d) (5,5) SWCNTs. Numbers of platinum atoms on free Pt_4 and Pt_4-decorated SWCNTs are labeled for their selected geometries comparison.

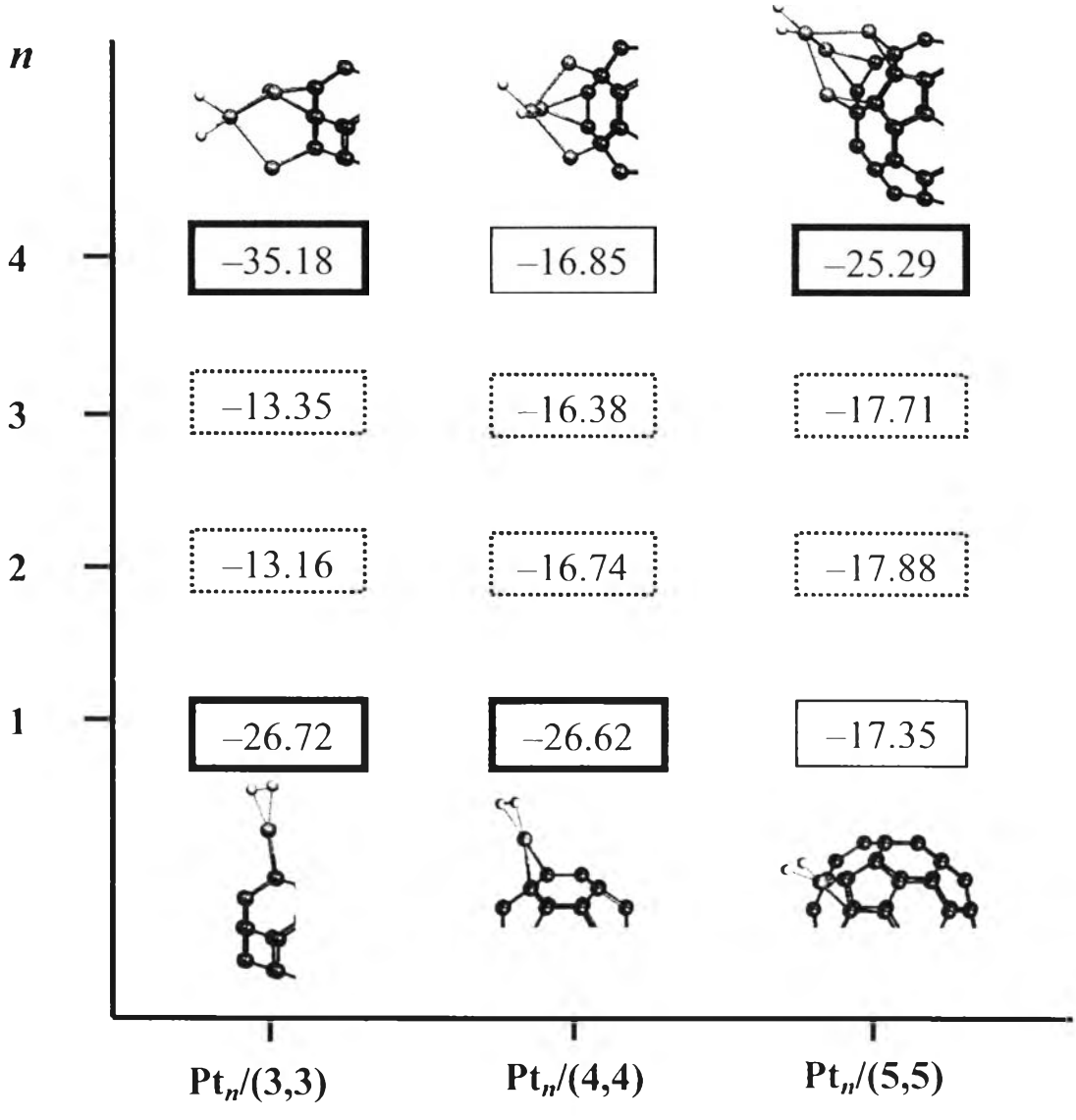

Figure A4. Adsorption energy (kcal/mol) diagram of hydrogen molecule on platinum atom of Pt_n decorated (3,3), (4,4) and (5,5) SWCNTs plotted against numbers (n) of platinum atom(s) of Pt_n clusters on SWCNTs. Strong adsorption structures are shown near their adsorption energies values in bold solid-line boxes; weak adsorption structures are in thin solid-line boxes.

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