

ภาคผนวก ก
การวิเคราะห์ข้อมูล

ตารางภาคผนวกที่ 1 จำนวนพลังงานการยึดจับและพลังงานการดูดซับ

ระบบ	SWCNT หรือ TM-SWCNT	โลหะ หรือ แก๊ส	TM-หรือ gas/ TM-SWCNT	ΔE_{ads} (amu.)	ΔE_{ads} (kcal/mol)
Sc-SWCNT	-3402.809	-46.363	-3449.432	-0.260	-163.377
Ti-SWCNT	-3402.809	-57.908	-3461.049	-0.332	-208.058
V-SWCNT	-3402.809	-71.158	-3474.277	-0.310	-194.395
Cr-SWCNT	-3402.809	-85.815	-3489.207	-0.583	-365.867
Mn-SWCNT	-3402.809	-103.752	-3506.856	-0.294	-184.726
Y-SWCNT	-3402.809	-37.848	-3440.909	-0.252	-157.921
Zr-SWCNT	-3402.809	-46.383	-3449.537	-0.345	-216.481
Nb-SWCNT	-3402.809	-56.104	-3459.267	-0.354	-222.190
Mo-SWCNT	-3402.809	-67.249	-3470.462	-0.404	-253.449
Tc-SWCNT	-3402.809	-79.835	-3483.037	-0.393	-246.755
NH ₃ /SWCNT	-3441.157	-56.548	-3497.706	-0.001	-0.7213
PH ₃ /SWCNT	-3441.157	-8.270	-3449.428	-0.001	-0.5148
AsH ₃ /SWCNT	-3441.157	-7.834	-3448.992	-0.001	-0.340
NH ₃ /Sc-SWCNT	-3449.432	-56.548	-3506.028	-0.048	-29.808
PH ₃ /Sc-SWCNT	-3449.432	-8.270	-3457.725	-0.023	-14.473
AsH ₃ /Sc-SWCNT	-3449.432	-7.834	-3457.347	-0.080	-50.320
NH ₃ /Ti-SWCNT	-3461.049	-56.548	-3517.655	-0.058	-36.236
PH ₃ /Ti-SWCNT	-3461.049	-8.270	-3469.349	-0.030	-18.627
AsH ₃ /Ti-SWCNT	-3461.049	-7.834	-3468.969	-0.086	-54.192
NH ₃ /V-SWCNT	-3474.277	-56.548	-3530.880	-0.054	-34.142
PH ₃ /V-SWCNT	-3474.277	-8.270	-3482.585	-0.039	-24.159
AsH ₃ /V-SWCNT	-3474.277	-7.834	-3482.206	-0.095	-59.754
NH ₃ /Cr-SWCNT	-3489.207	-56.548	-3545.815	-0.059	-37.163
PH ₃ /Cr-SWCNT	-3489.207	-8.270	-3497.513	-0.036	-22.562
AsH ₃ /Cr-SWCNT	-3489.207	-7.834	-3497.134	-0.092	-58.291

ตารางภาคผนวกที่ 2 จำนวนแถบพลังงาน

ระบบ	E_{HOMO} (au)	E_{HOMO} (eV)	E_{LUMO} (au)	E_{LUMO} (eV)	E_{gap} (eV)	ΔE_{gap} (eV)
SWCNT	-0.162	-4.408	-0.121	-3.293	1.116	-
Sc-SWCNT	-0.147	-4.000	-0.104	-2.830	1.170	-0.054
Ti-SWCNT	-0.152	-4.136	-0.112	-3.048	1.088	0.027
V-SWCNT	-0.166	-4.517	-0.117	-3.184	1.333	-0.218
Cr-SWCNT	-0.160	-4.354	-0.118	-3.211	1.143	-0.027
Mn-SWCNT	-0.145	-3.946	-0.102	-2.776	1.170	-0.054
Y-SWCNT	-0.145	-3.946	-0.102	-2.776	1.170	-0.054
Zr-SWCNT	-0.149	-4.055	-0.110	-2.993	1.061	0.054
Nb-SWCNT	-0.154	-4.191	-0.122	-3.320	0.871	0.245
Mo-SWCNT	-0.158	-4.300	-0.124	-3.374	0.925	0.190
Tc-SWCNT	-0.164	-4.463	-0.116	-3.157	1.306	-0.190
NH ₃ /SWCNT	-0.163	-4.436	-0.122	-3.320	1.116	-
NH ₃ /Cr-SWCNT	-0.151	-4.109	-0.110	-2.993	1.116	0.000
NH ₃ /Sc-SWCNT	-0.140	-3.810	-0.097	-2.640	1.170	-0.054
NH ₃ /Ti-SWCNT	-0.144	-3.919	-0.104	-2.830	1.088	0.027
NH ₃ /V-SWCNT	-0.146	-3.973	-0.108	-2.940	1.034	0.082
PH ₃ /SWCNT	-0.163	-4.436	-0.122	-3.320	1.116	-
PH ₃ /Cr-SWCNT	-0.156	-4.245	-0.113	-3.075	1.170	-0.054
PH ₃ /Sc-SWCNT	-0.142	-3.864	-0.099	-2.694	1.170	-0.054
PH ₃ /Ti-SWCNT	-0.146	-3.973	-0.106	-2.885	1.088	0.027
PH ₃ /V-SWCNT	-0.146	-3.973	-0.104	-2.830	1.143	-0.027
AsH ₃ /SWCNT	-0.162	-4.408	-0.120	-3.265	1.143	-
AsH ₃ /Cr-SWCNT	-0.157	-4.272	-0.114	-3.102	1.170	-0.027
AsH ₃ /Sc-SWCNT	-0.143	-3.891	-0.099	-2.694	1.197	-0.054
AsH ₃ /Ti-SWCNT	-0.147	-4.000	-0.107	-2.912	1.088	0.054
AsH ₃ /V-SWCNT	-0.147	-4.000	-0.105	-2.857	1.143	0.000