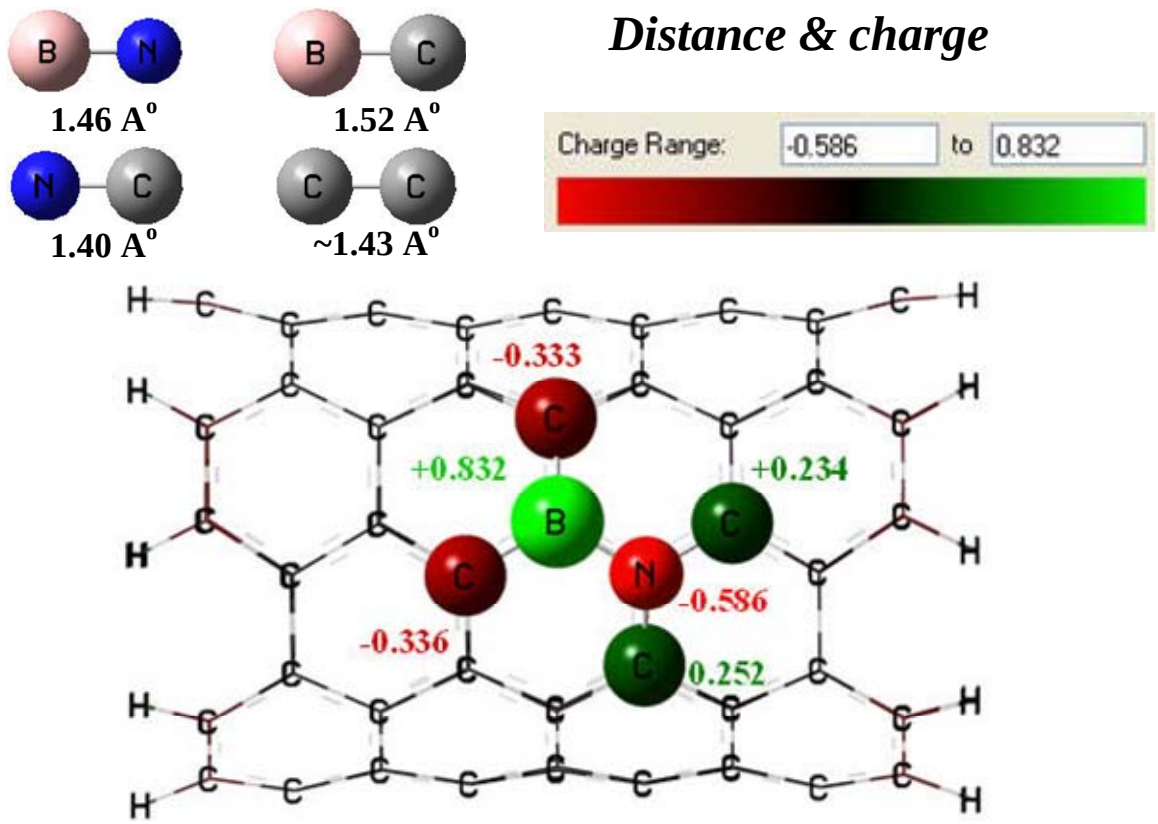

Figure 9 Bond lengths and charge distribution of BN-doped (5,5)SWCNT

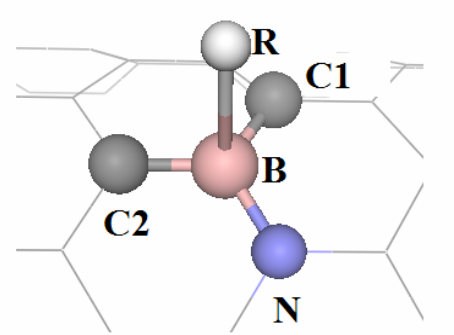

Figure 10 Position of R groups, B atom, N atom, C1 atom, C2 atom on side-wall (5,5) SWCNT

Table 2 Structural parameters of BN-doped SWCNT grafted with N-nucleophiles

	R-B	B-N	B-C1	B-C2	∠N-B-C1	∠N-B-C2	∠C1-B-C2	∠R-B-N	∠R-B-C1	∠R-B-C2
BN-SWCNT	-	1.46	1.53	1.51	118.0	118.6	114.7	-	-	-
m-nitroaniline	1.79	1.52	1.59	1.57	111.8	113.8	110.0	105.1	108.3	107.5
pyridine	1.67	1.54	1.60	1.58	109.9	112.0	108.3	105.7	112.1	108.9
chitosan	1.70	1.54	1.61	1.58	109.3	112.1	107.3	106.5	112.2	109.2
imidazole	1.64	1.55	1.60	1.59	109.7	111.9	108.0	106.6	111.0	109.7
ammonia	1.69	1.54	1.60	1.58	110.8	112.9	109.0	105.9	109.6	108.5
arginine	1.60	1.57	1.61	1.59	108.3	110.4	107.2	107.2	110.4	113.3
guanidine	1.61	1.57	1.61	1.59	108.2	110.5	107.0	108.2	109.6	113.2

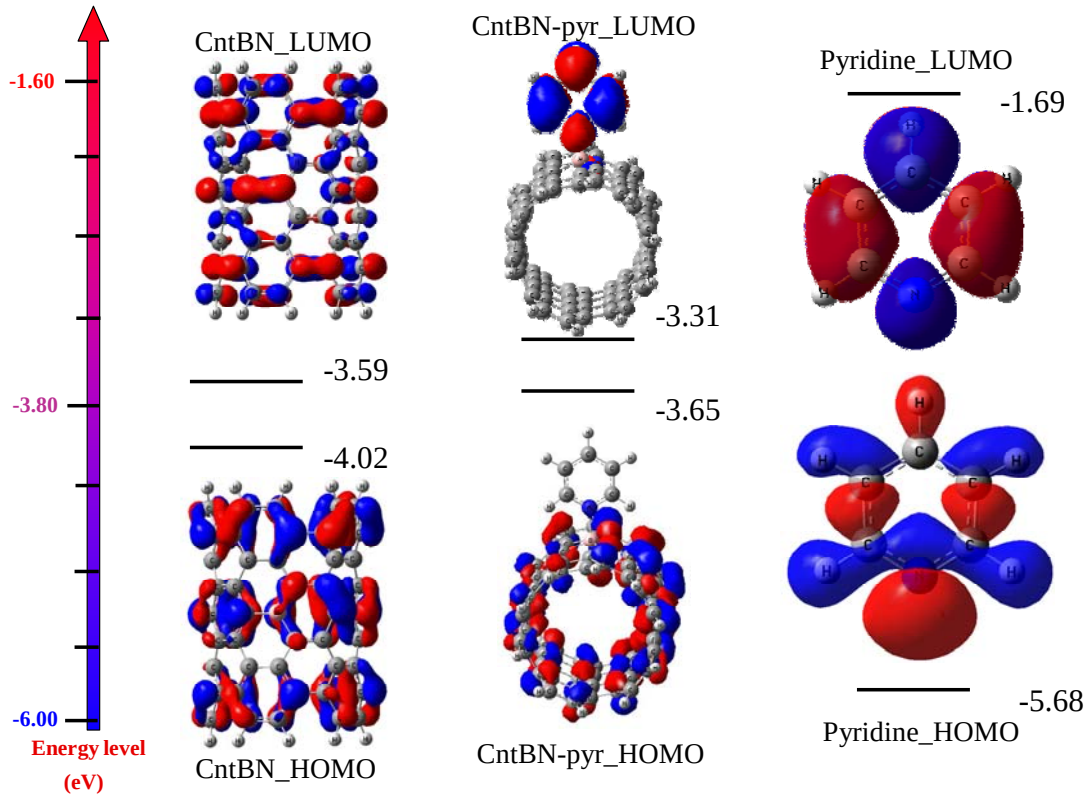

Figure 17 HOMO and LUMO orbital energies of isolated pyridine and pyridine complexed with BN-doped SWCNT

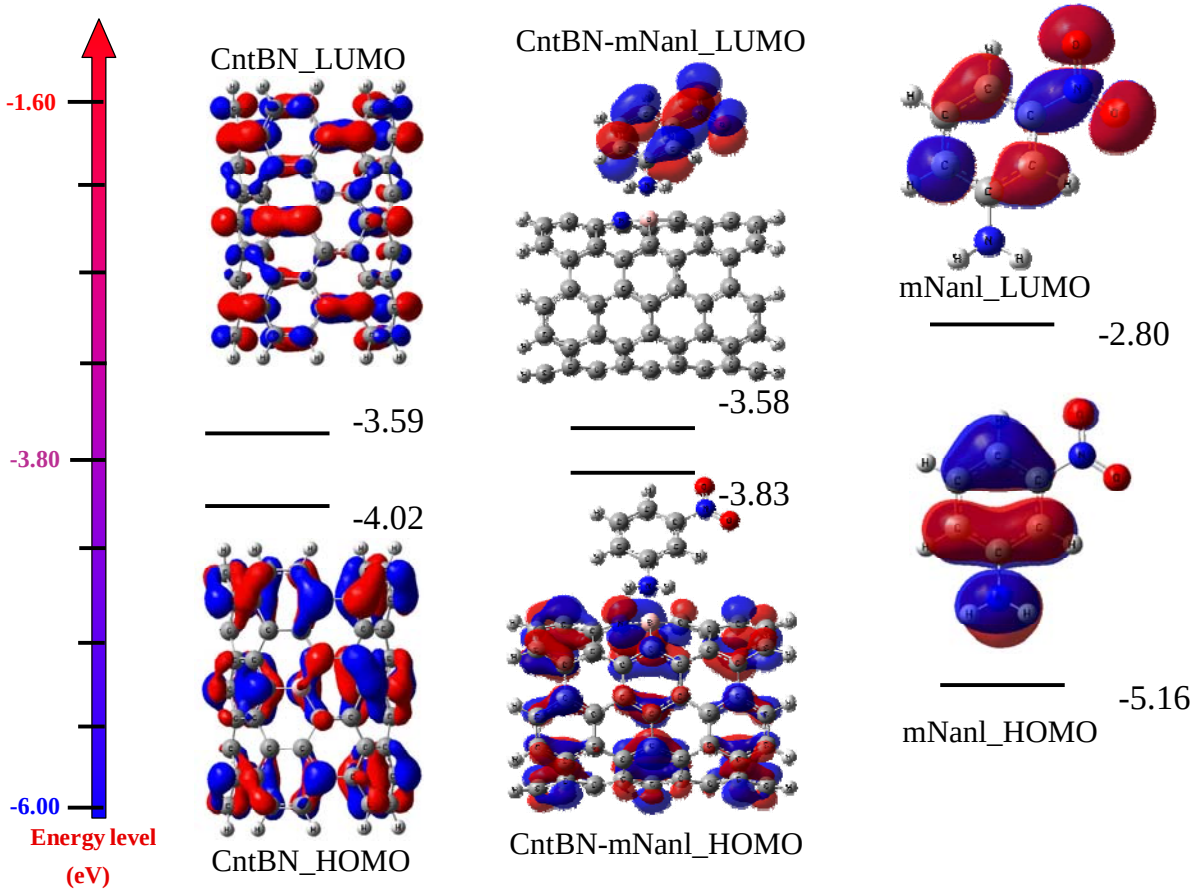

Figure 18 HOMO and LUMO orbital energies of isolated m-nitroaniline and m-nitroaniline complexed with BN-doped SWCNT

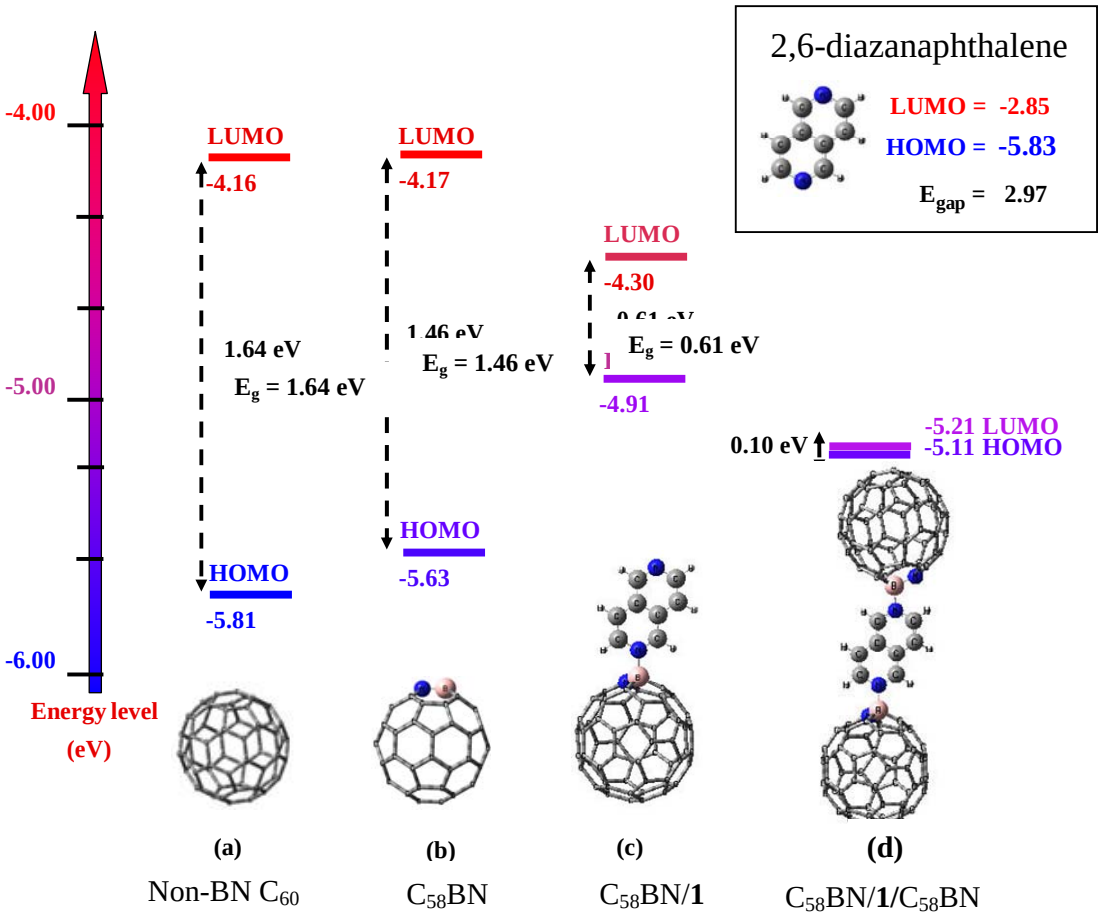

Figure 19 HOMO and LUMO orbital energies and energy gap of isolated 2,6-diazanaphthalene (**1**) and $C_{58}BN$/**1**/$C_{58}BN$ complex

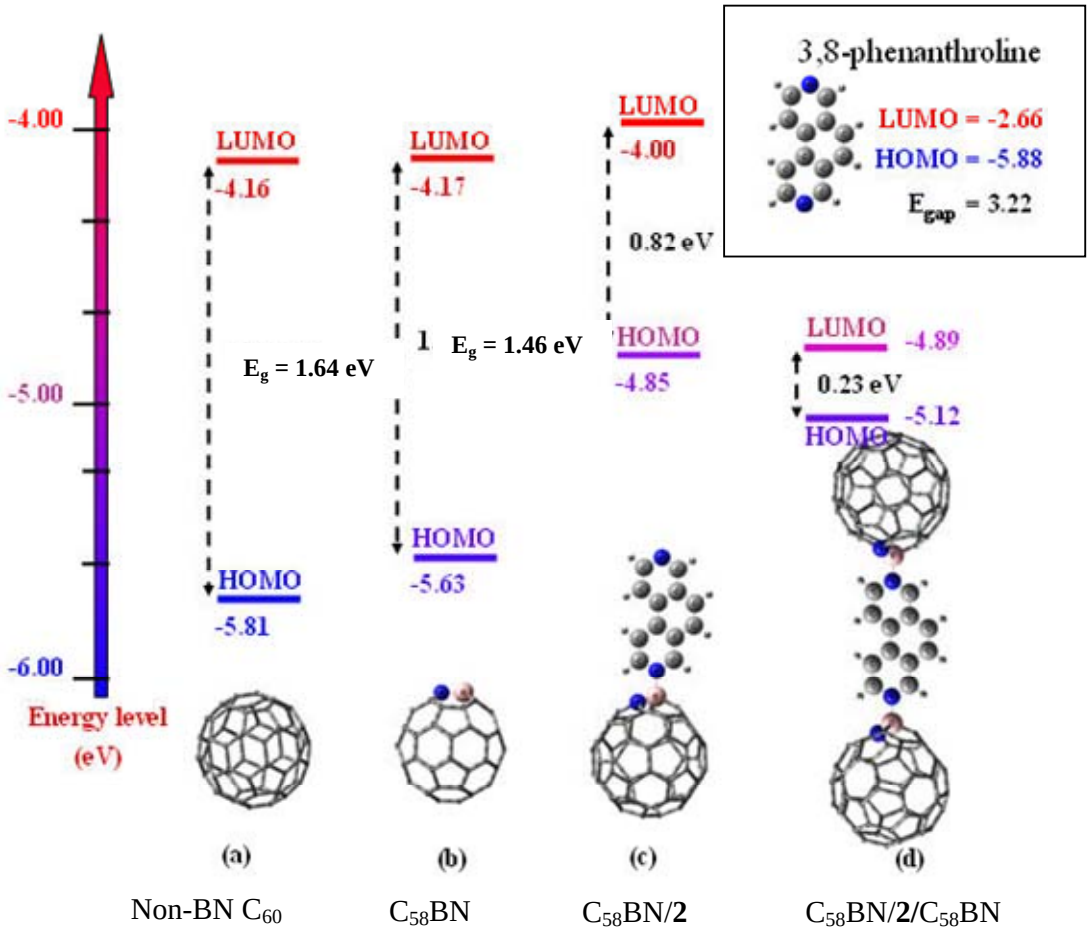

Figure 20 HOMO and LUMO orbital energies and energy gap of isolated 3,8-phenanthroline (**2**) and $C_{58}BN$/**2**/$C_{58}BN$ complex

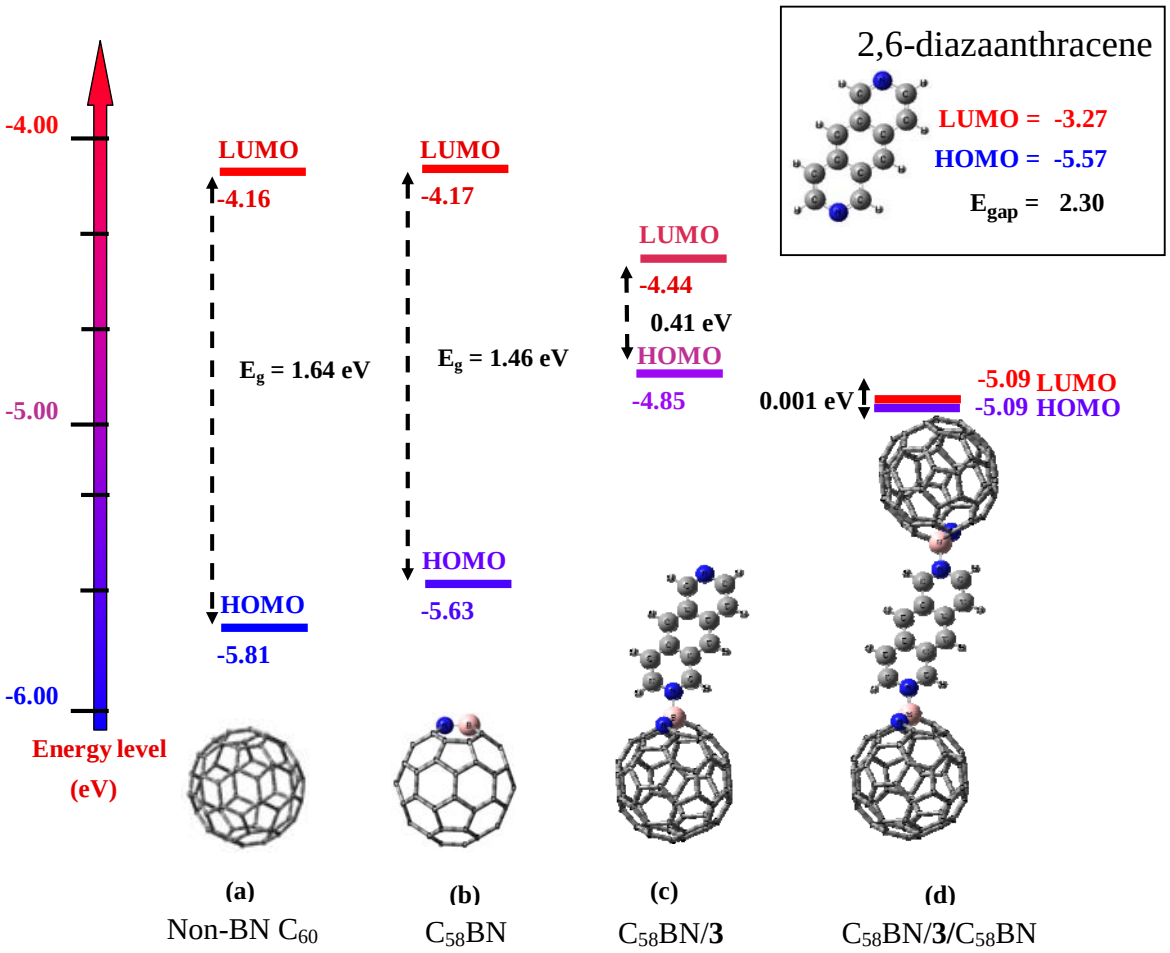

Figure 21 HOMO and LUMO orbital energies and energy gap of isolated 2,6- diazaanthracene (**3**) and $C_{58}BN$/**3**/$C_{58}BN$ complex