

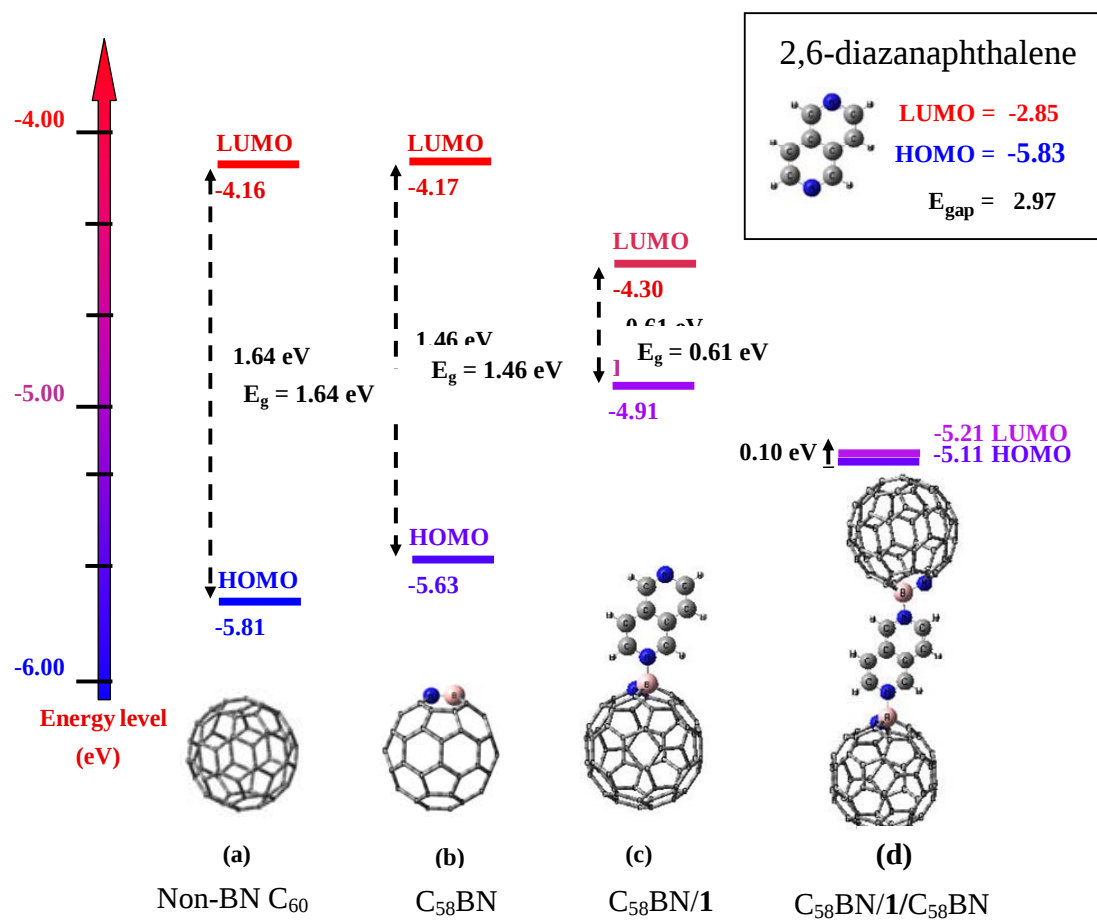


Figure 19 HOMO and LUMO orbital energies and energy gap of isolated 2,6-diazanaphthalene (1) and C₅₈BN/1/C₅₈BN complex