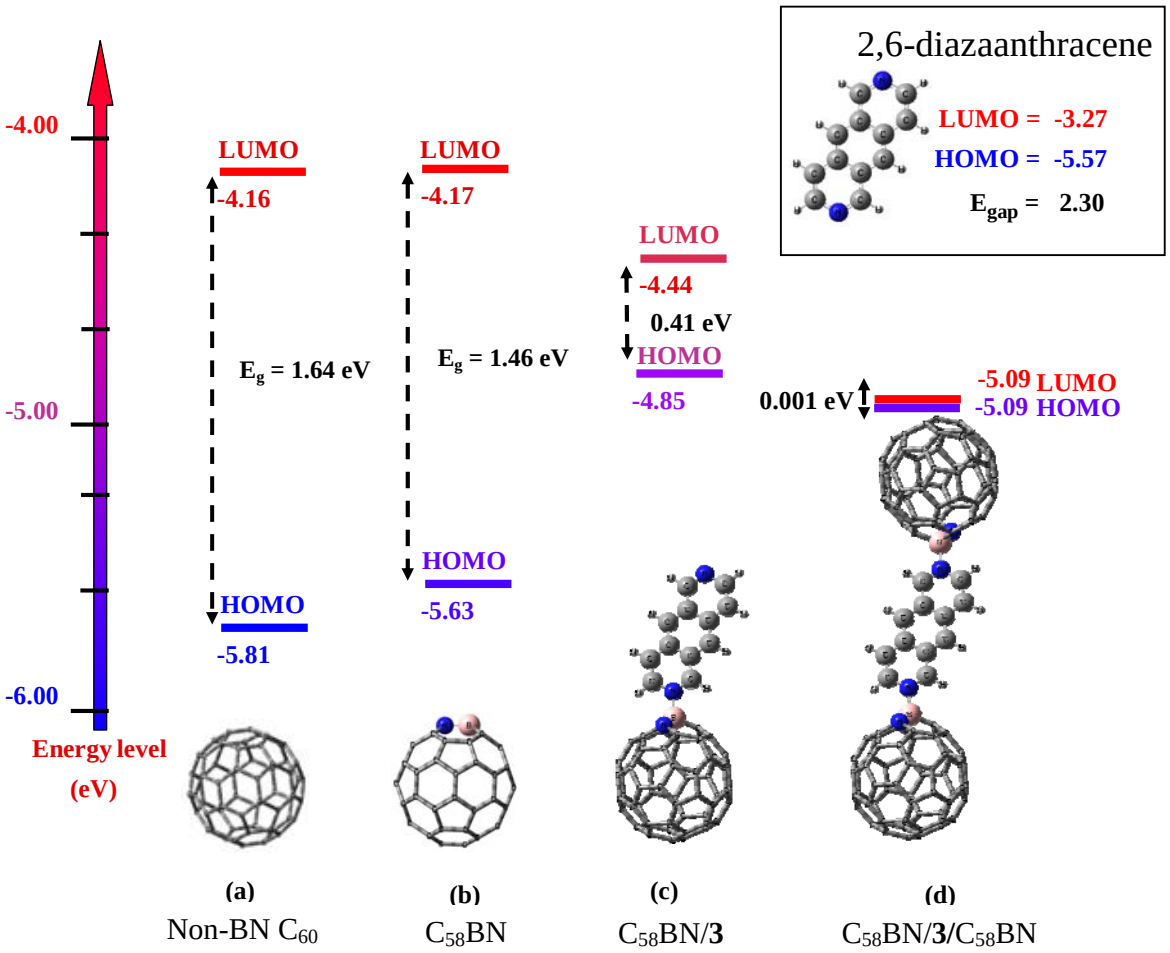

Figure 21 HOMO and LUMO orbital energies and energy gap of isolated 2,6- diazaanthracene (**3**) and $C_{58}BN$/**3**/$C_{58}BN$ complex