

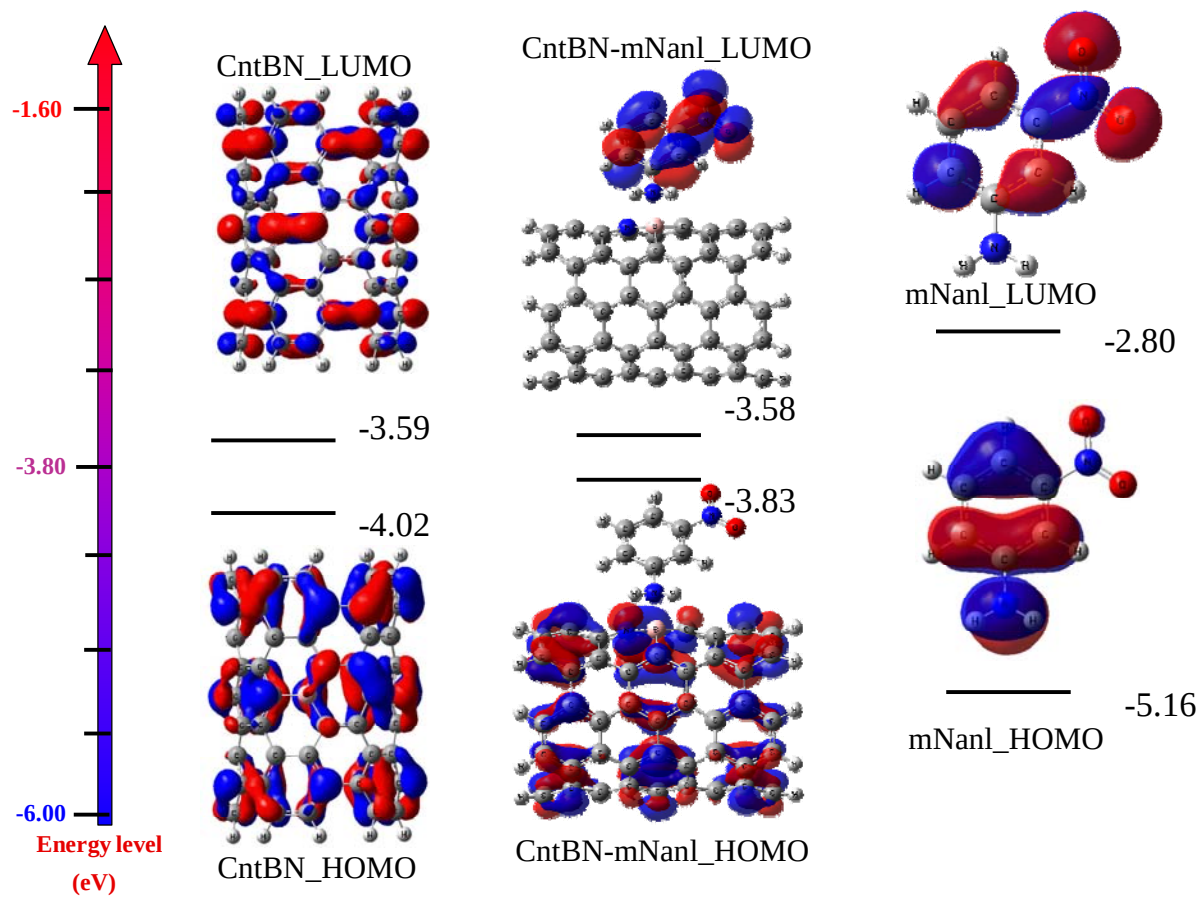


Figure 18 HOMO and LUMO orbital energies of isolated m-nitroaniline and m-nitroaniline complexed with BN-doped SWCNT