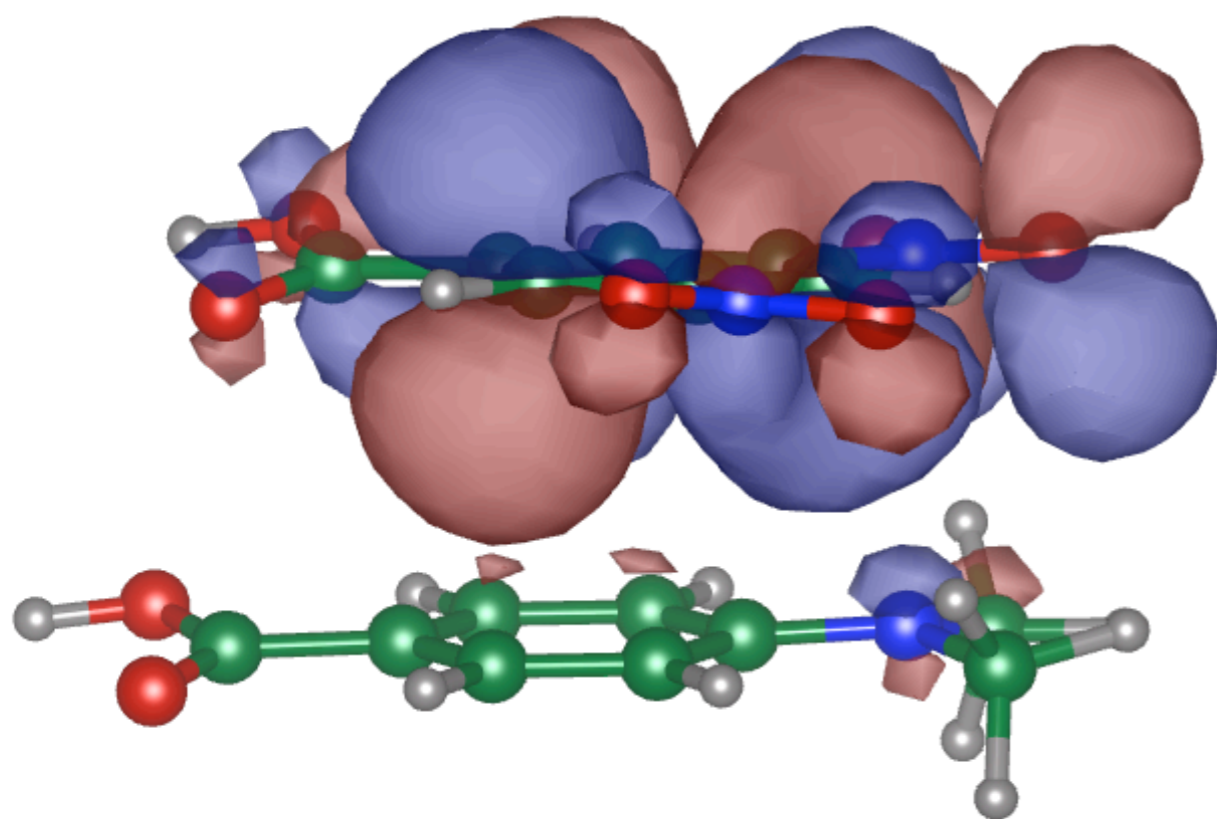
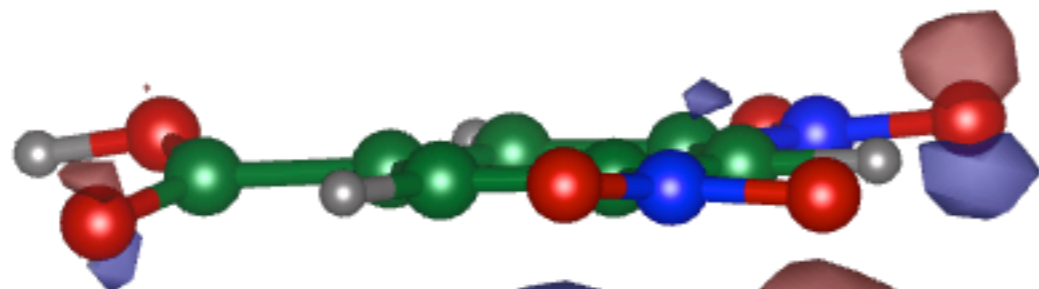


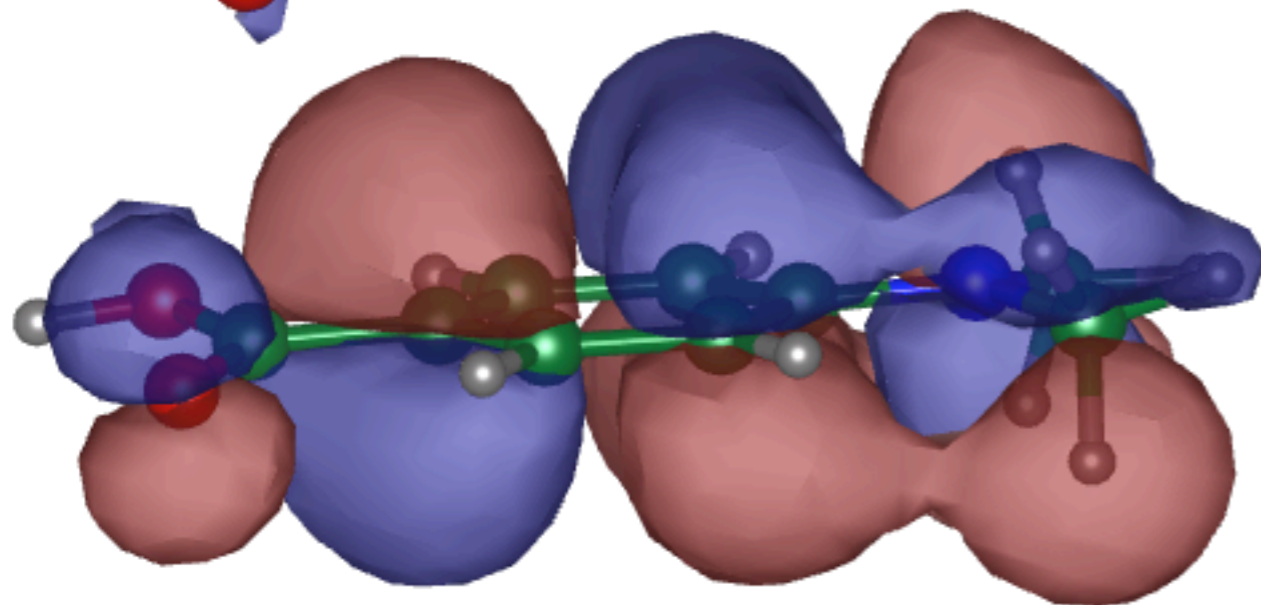
# Neutral Dimer System



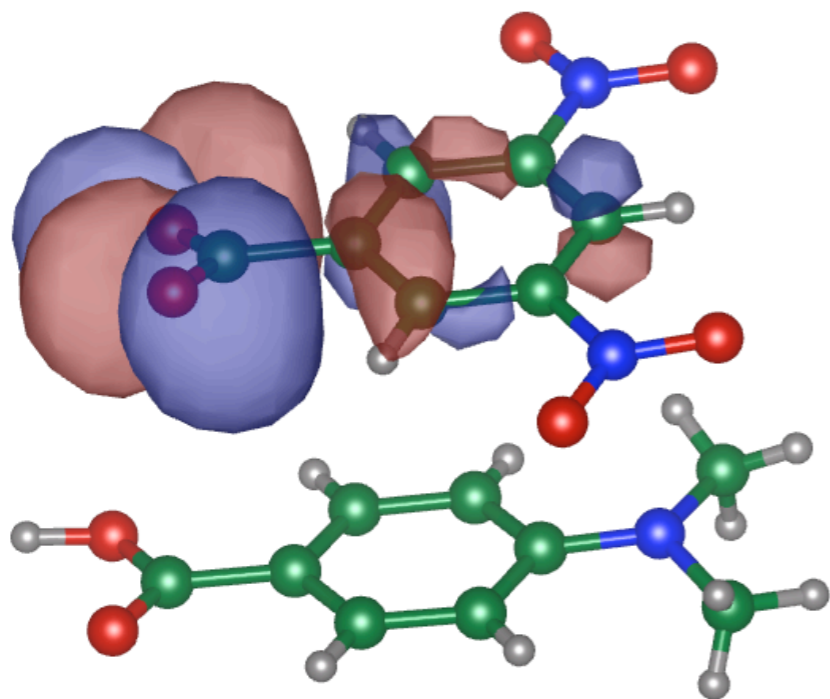
LUMO of 3,5-dnba/  
4-dmaba dimer  
 $E = -1.9118 \text{ eV}$



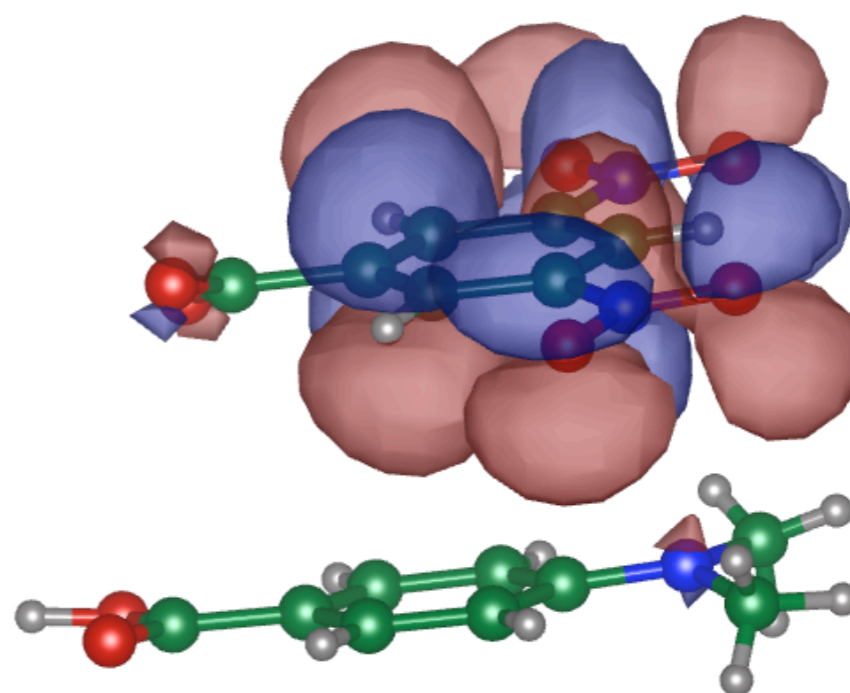
HOMO of 3,5-dnba/  
4-dmaba dimer  
 $E = -7.056 \text{ eV}$



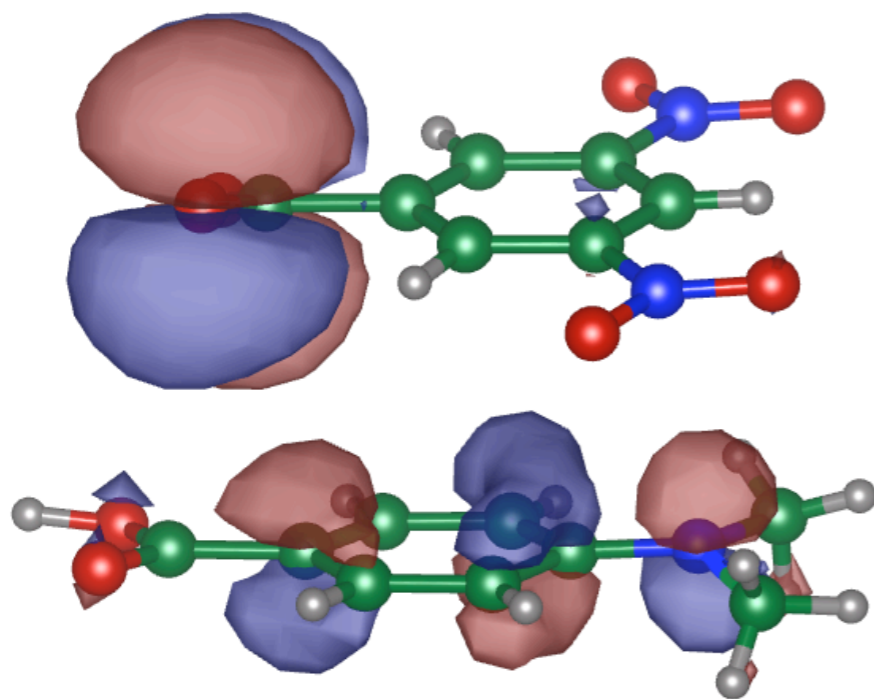
# 1<sup>-</sup> Dimer System



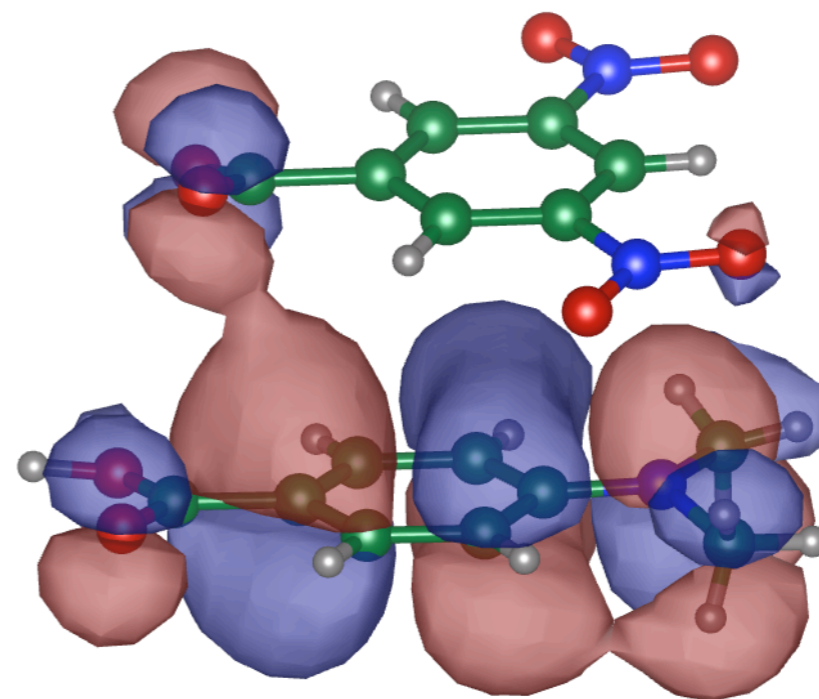
LUMO of 3,5-dnba-/4-dmaba dimer  
E = 1.1755 eV



HOMO of 3,5-dnba-/4-dmaba dimer  
E = -3.9981 eV

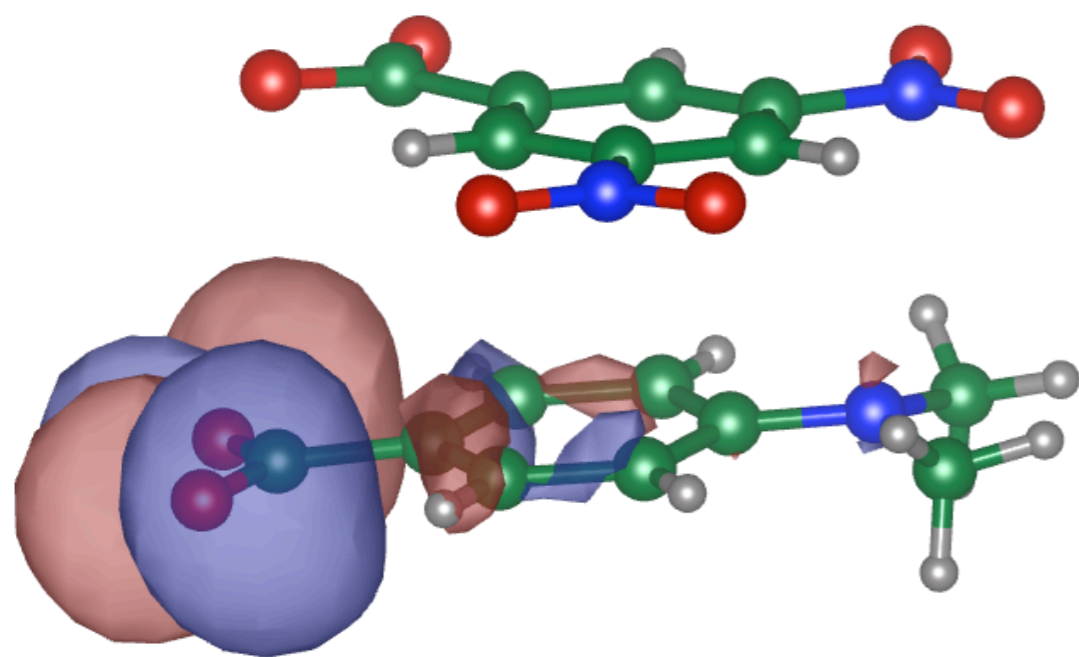


2<sup>nd</sup> HOMO of 3,5-dnba-/4-dmaba dimer  
E = -4.0582 eV

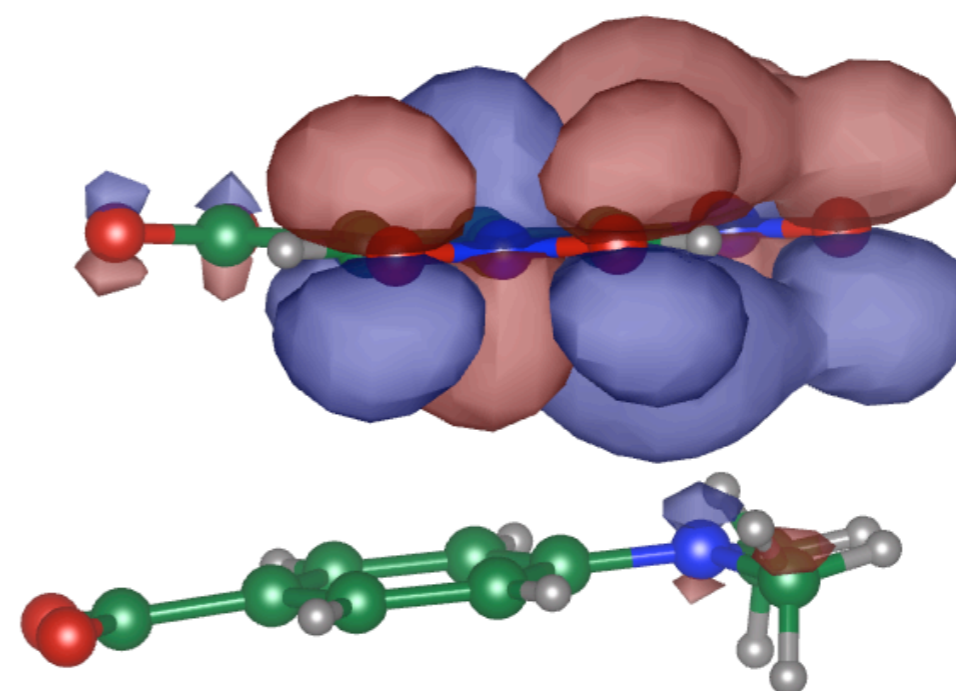


3<sup>rd</sup> HOMO of 3,5-dnba-/4-dmaba dimer  
E = -4.1625 eV

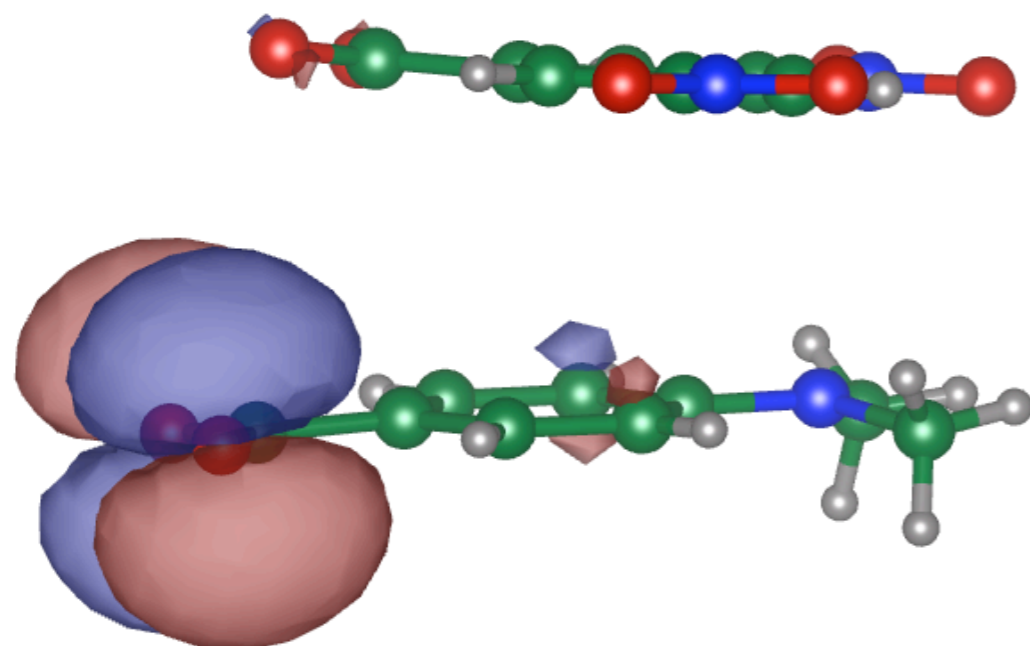
# 2<sup>-</sup> Dimer System



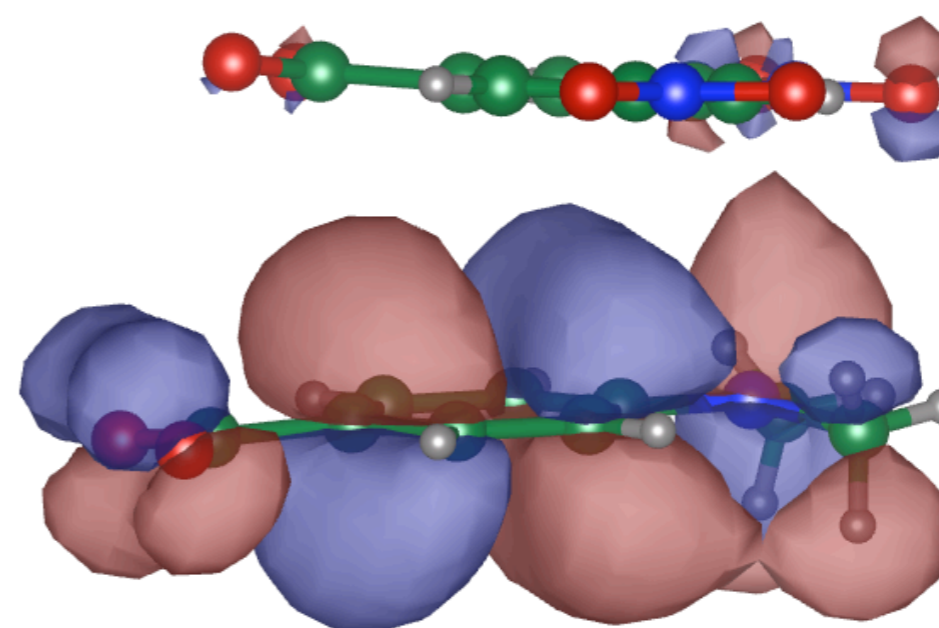
LUMO of 3,5-dnba<sup>-</sup>/4-dmaba<sup>-</sup> dimer  
E = 3.5366 eV



HOMO of 3,5-dnba<sup>-</sup>/4-dmaba<sup>-</sup> dimer  
E = -0.1239 eV



2<sup>nd</sup> HOMO of 3,5-dnba<sup>-</sup>/4-dmaba<sup>-</sup> dimer  
E = -0.246 eV



3<sup>rd</sup> HOMO of 3,5-dnba<sup>-</sup>/4-dmaba<sup>-</sup> dimer  
E = -0.6176 eV