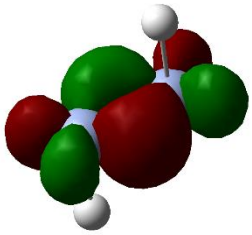
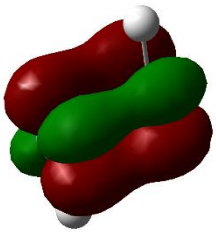
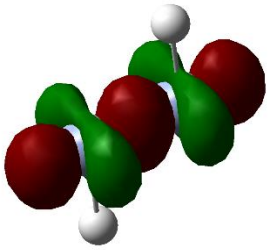
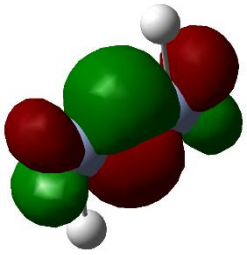
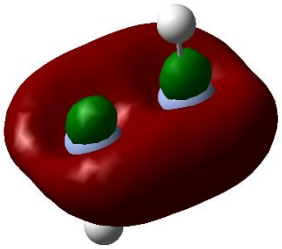
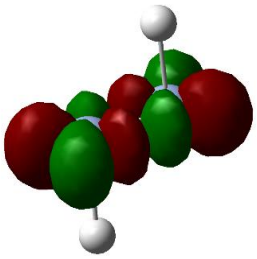
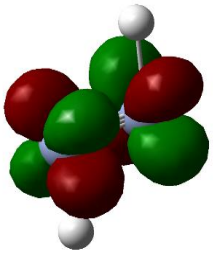
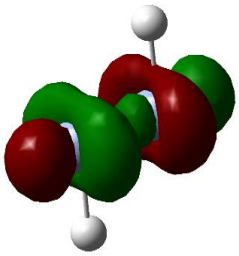
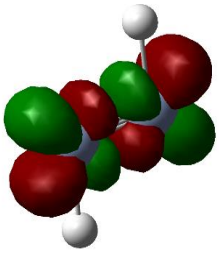
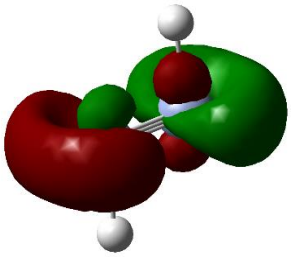
計算生物（二）第八周作業

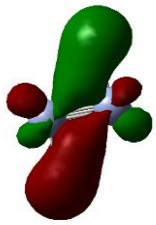
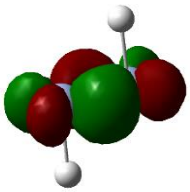
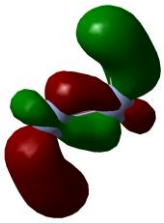
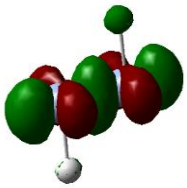
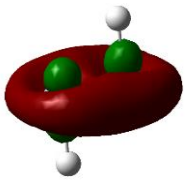
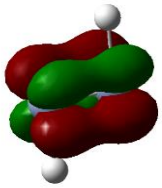
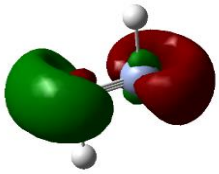
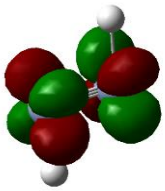
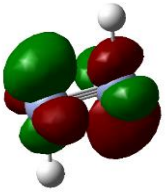
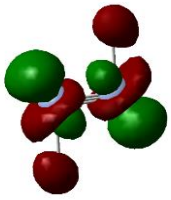
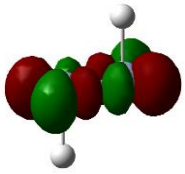
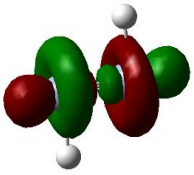
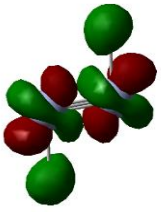
0317033 謝明修

1. Find out all Cr—Cr bonding orbital in H—Cr—Cr—H and calculate the bond order, using NBO and CMO

NBO:

 π d_{xz}	 δ d_{xy}
 σ d_z^2	 δ d_{yz}
 δ s+ $d_{x^2-y^2}$	 π* d_{xz}
 δ* d_{xy}	 σ* d_z^2
 δ* d_{yz}	 δ* s+ $d_{x^2-y^2}$

CMO:

 $\pi\ d_{xz} + \sigma_{Cr—H}$	 $\pi\ d_{xz}$
 $\pi\ d_{xz} + \sigma_{Cr—H}$	 $\sigma\ d_z^2 + \text{H core orbital}$
 $\delta\ s + d_{x^2-y^2}$	 $\delta\ d_{xy}$
 $\delta^*\ s + d_{x^2-y^2}$	 $\delta^*\ d_{xy}$
 $\delta^*\ d_{xy}$	 $\delta^*\ d_{yz} + \text{H core orbital}$
 $\pi^*\ d_{xz}$	 $\sigma^*\ d_z^2$
 $\delta^*\ d_{yz} + \text{H core orbital}$	

2. Calculate the first excitation energy and emission energy for poly (p-phenylene vinylene) (PPV) at the level of B3LYP/6-31G(d).

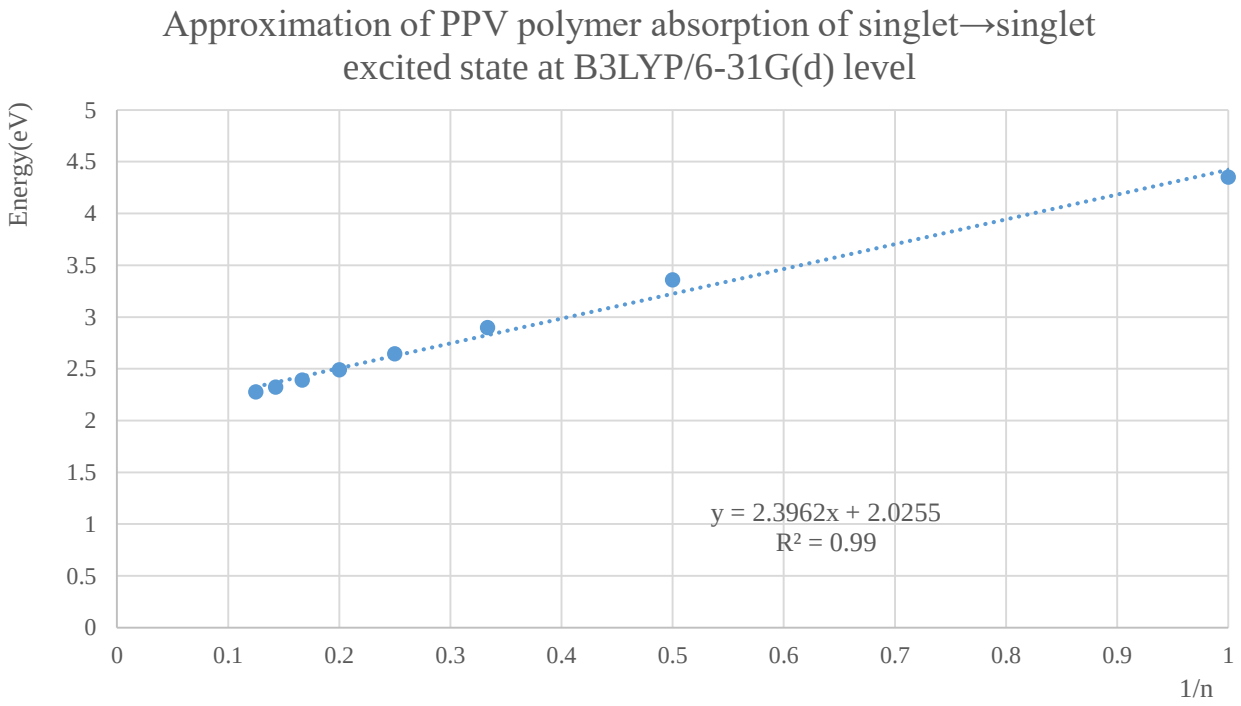


Figure1. At each length of PPV, calculating the absorption energy and plot in figure. The Y-intercept is the approximate absorption energy (2.0255eV).

B3LYP/6-31G(d)	
Number of monomer (n)	Excitation energy(eV)
1	4.3489
2	3.3567
3	2.8969
4	2.6424
5	2.4876
6	2.3884
7	2.3212
Approximate excitation energy (eV)	2.0255
Wavelength (nm)	612.34

Table 1. The energy at each length of PPV.

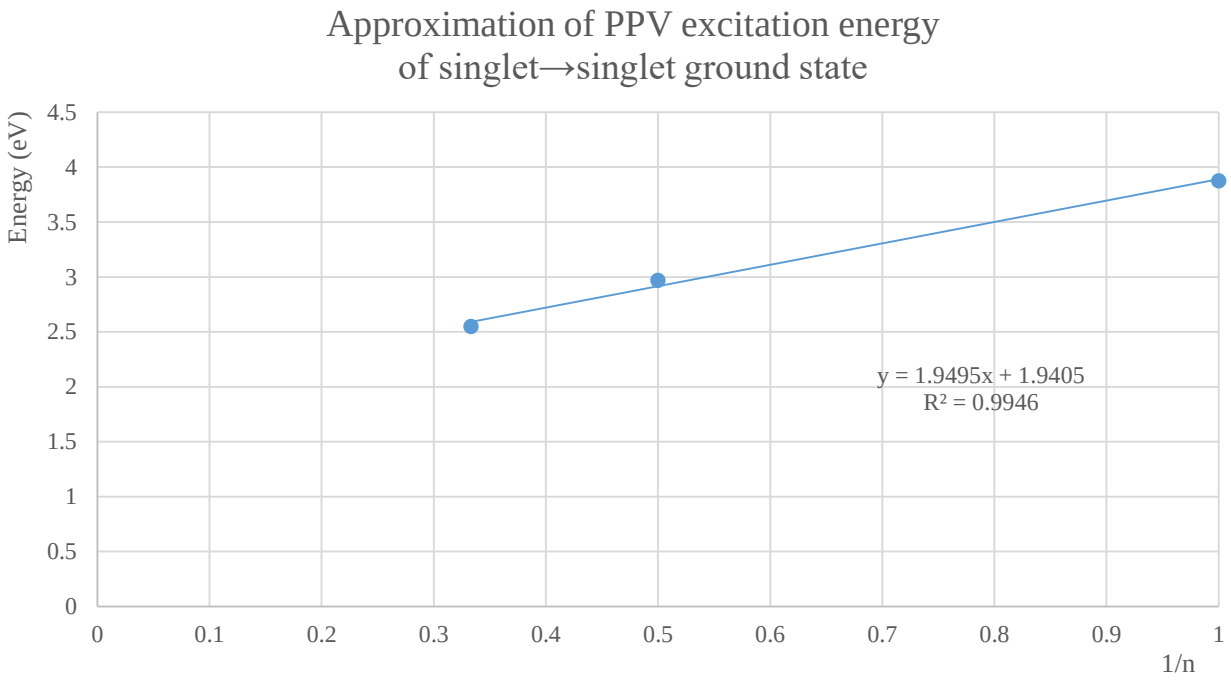


Figure2. At each length of PPV, calculating the emission energy and plot in figure. The Y-intercept is the approximate emission energy (1.9405eV).

B3LYP/6-31G(d)	
Number of monomer (n)	Excitation energy(eV)
1	3.8761
2	2.9707
3	2.5487
Approximate excitation energy (eV)	1.9405
Wavelength (nm)	639.01
Stoke shift(nm)	26.67

Table 2. The energy at each length of PPV.