粒線體產能機制之量子生物分析

Quantum Biology Analysis of the Energy Generation Mechanism for Mitochondria

Department of Power Mechanical Engineering, National Tsing Hua University

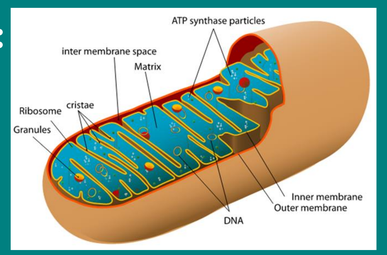
Wan-Ning Lee(李婉寧) (Research student), Che-Wun Hong (洪哲文) (Professor)

Green Energy & Quantum Engineering Lab

◆Objective

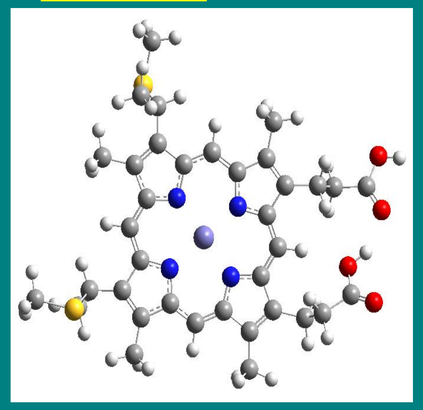
- To setup the optimized structure and to compute the thermochemical energy of the cytochrome c oxidase with different center molecular structure according to the electron transport procedure.

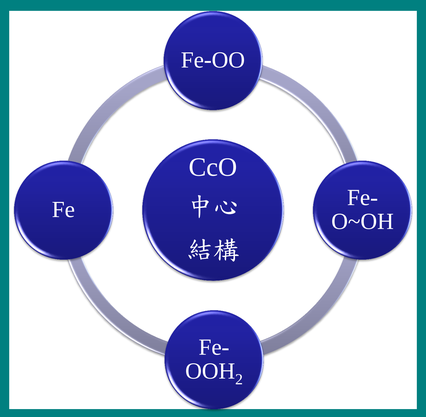
- Quantum simulation results:
  - Thermochemistry energy
  - HOMO & LUMO
  - Reaction rate and Activity



Ref: LadyofHats, M. R. V. Mitochondrion.Available from: http://commons.wikimedia.org/wiki/File:Animal_mitochondrion_diagram_en.svg.

◆Abstract





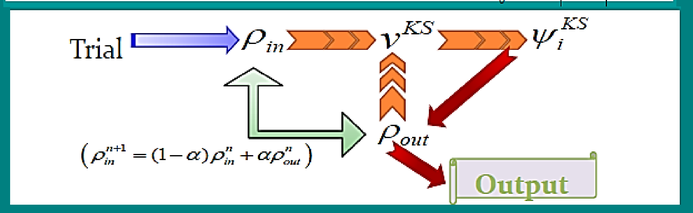
- This thesis mainly studies the electron transport mechanism of CcO by using density function theory（DFT） with the B3LYP/6-31G(d, p) exchange-correlation function.
- In this study, the functional models of the metallic active in CcO is simulated. Besides, thermochemistry data and reaction rate are discussed as well.

◆Theory : DFT(Density Functional Theory), SCF(Self-Consistent Field)

Kohn-Sham (KS) Equation

$$E^{KS}\psi^{KS}(\mathbf{r}) = \left[-\frac{\hbar^2}{2m}\nabla^2 + v^{KS}(\mathbf{r})\right]\psi^{KS}(\mathbf{r})$$

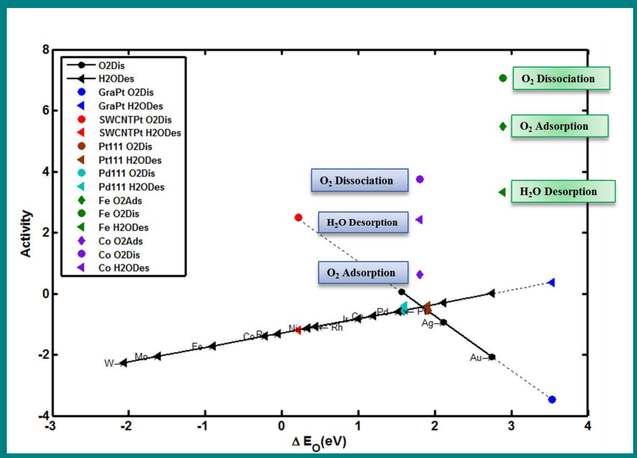
$$v^{KS}(\mathbf{r}) = v_{ext}(\mathbf{r}) + v_H(\mathbf{r}) + v_{xc}(\mathbf{r}) \qquad v_H := \frac{e^2}{4\pi\varepsilon_0}\int d^3r' \frac{1}{|\mathbf{r}-\mathbf{r}'|}\rho_0(\mathbf{r}')$$



◆Sabatier Analysis: rate (k) & activity (A)

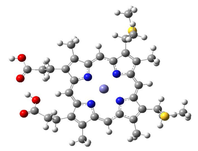
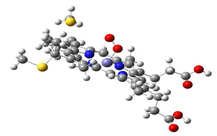
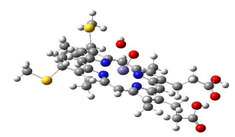
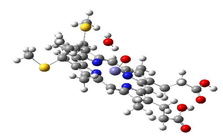
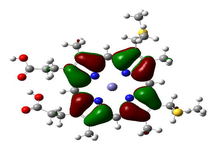
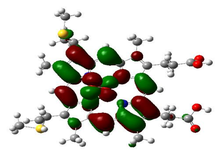
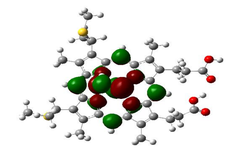
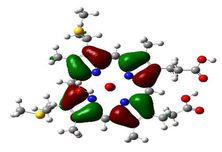
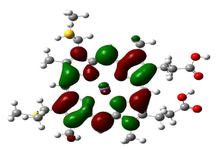
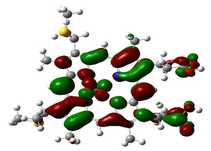
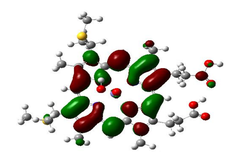
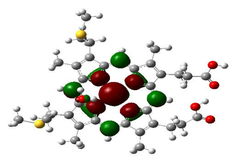
$$k(T) = \frac{k_B T}{h} e^{\frac{-\Delta G}{RT}} \qquad A = k_B T \min_i \left(\log\left(\frac{k_i}{k_o}\right)\right)$$

◆Reaction rate and activity



- The reaction rate and activity of the functional structure is higher than inorganic enzyme.

◆Structures and HOMO/LUMO

	Fe	Fe-OO	Fe-OOH	Fe-O~H_2O
Optimized structure				
HOMO				
LUMO				

- Both electron lost and obtainment mainly occur on the center of molecular structures.