Charge transport properties in organic electronics

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Outline

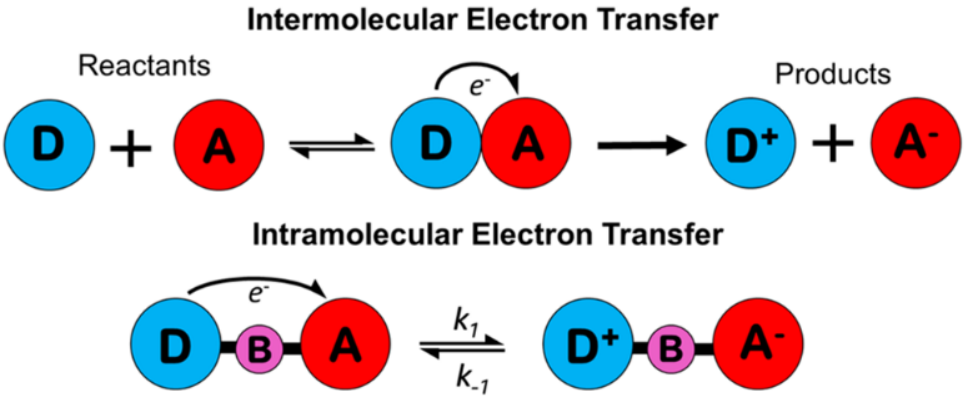
Introduction

- movement of charge carriers
- Carbon based material
- Eco-friendly and low cost
- flexibility

Main objectives

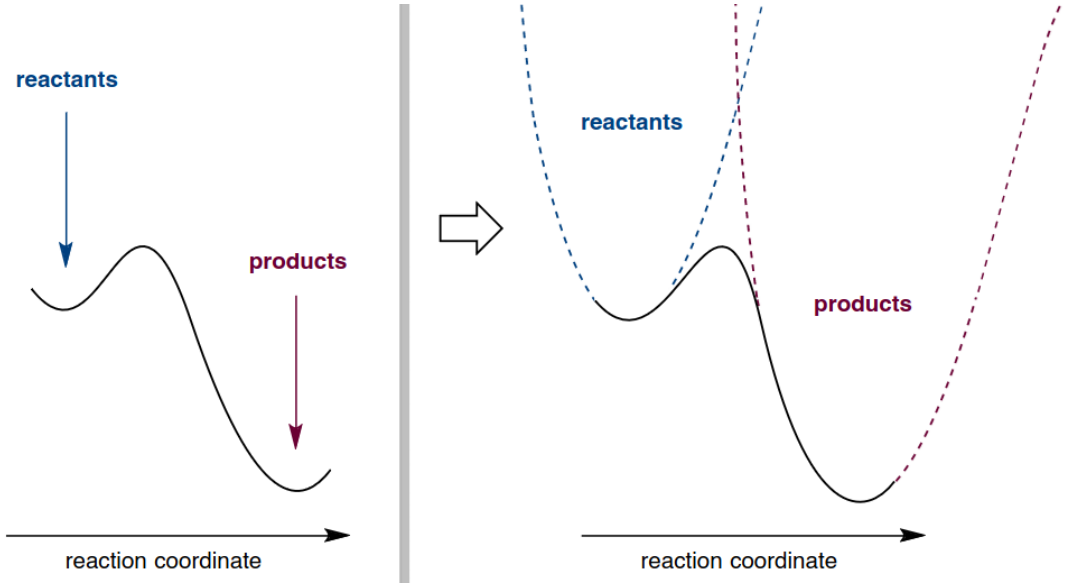
- The design,implementation,and testing of charge transfer models
- The design and implementation of a graphical user interface
- Quantum entanglement and correlation analysis

Electron transfer

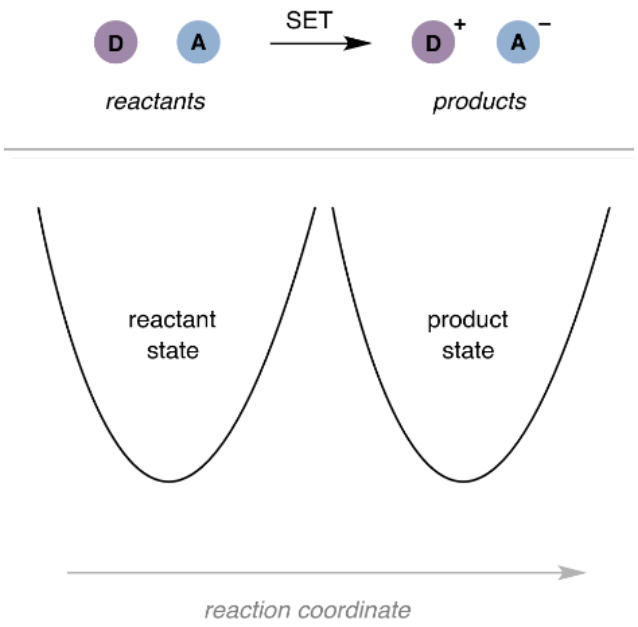


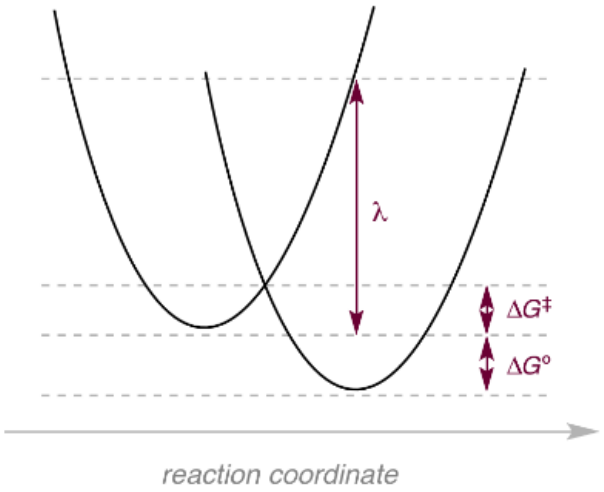
(Top):Formation of encounter complex
(Bottom):Rigid molecular bridge

Marcus theory



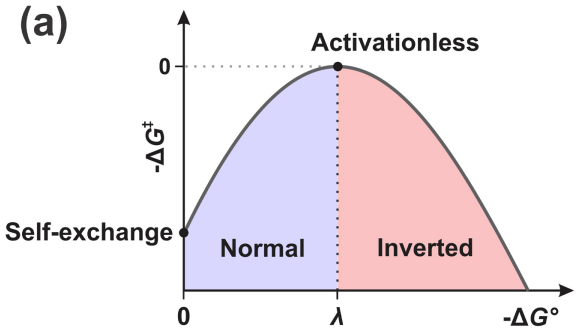
Marcus theory

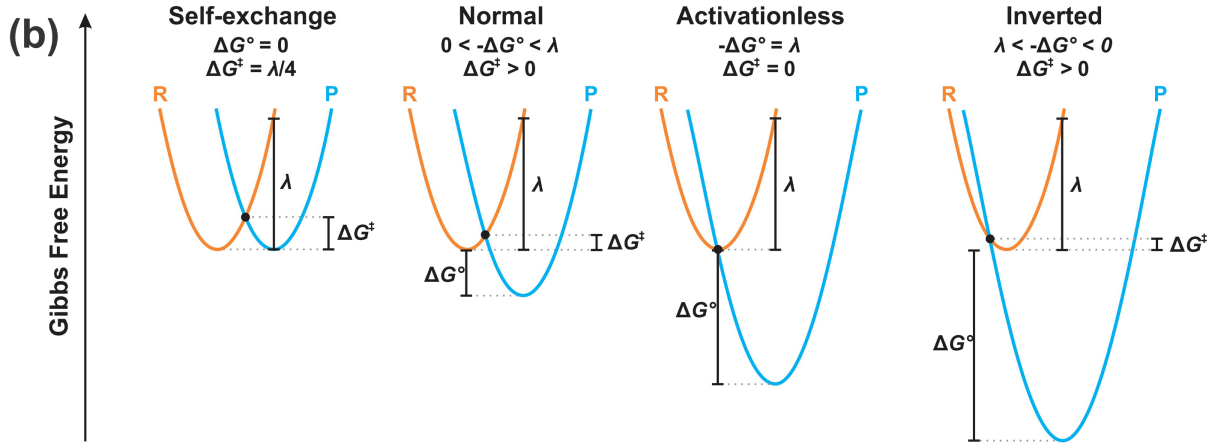




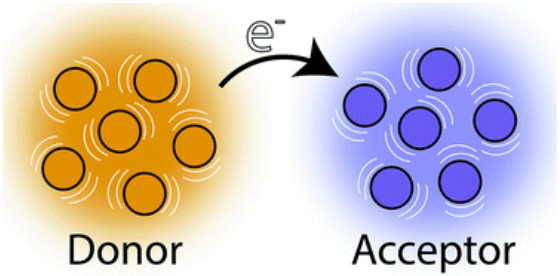
$$\Delta G^{\ddagger} = \frac{(\lambda + \Delta G^{\circ})^2}{4\lambda}$$

Marcus theory





Marcus-theory



The electron transfer rate..

$$k_{ET} = \frac{2\pi}{\hbar^2} t^2 \sqrt{\frac{1}{4\lambda\pi k_B T}} \exp\left[\frac{-\left(\Delta G^\circ + \lambda\right)^2}{4\lambda k_B T}\right]$$

controlled by $\Delta G^\circ, \lambda$, and t

Reorganization energy

The reorganization energy λ is defined as

$$\lambda = (E^{charged}_{neutralgeometry} - E^{neutral}_{neutralgeometry}) + (E^{neutral}_{chargedgeometry} - E^{charged}_{chargedgeometry})$$

$$\lambda = \lambda_1 + \lambda_2$$

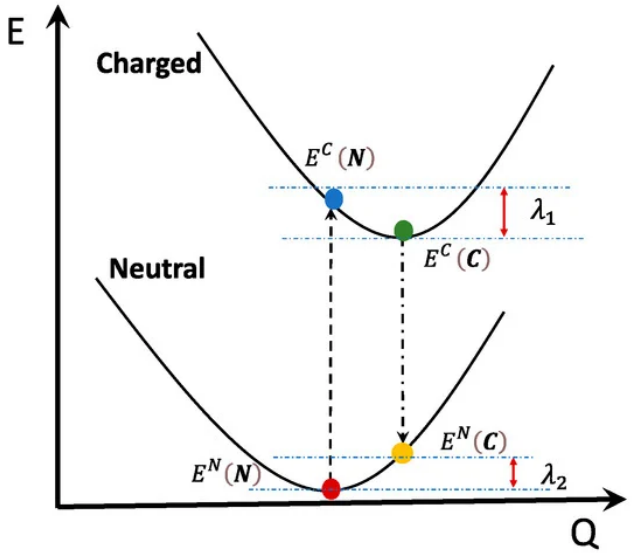


Figure 1: Adiabatic potential energy curves

Charge transfer integral

$$V = \frac{J - S(e1 + e2)/2}{1 - S^2} - -- > (a)$$

$$J = \left\langle \phi_1 \left| \hat{H} \right| \phi_2 \right\rangle - -- > (b)$$

$$S = \langle \phi_1 \mid \phi_2 \rangle - -- > (c)$$

$$e_1 = \left\langle \phi_1 \left| \hat{H} \right| \phi_1 \right\rangle - -- > (d)$$

$$e_2 = \left\langle \phi_2 \left| \hat{H} \right| \phi_2 \right\rangle - -- > (e)$$

ESID Method

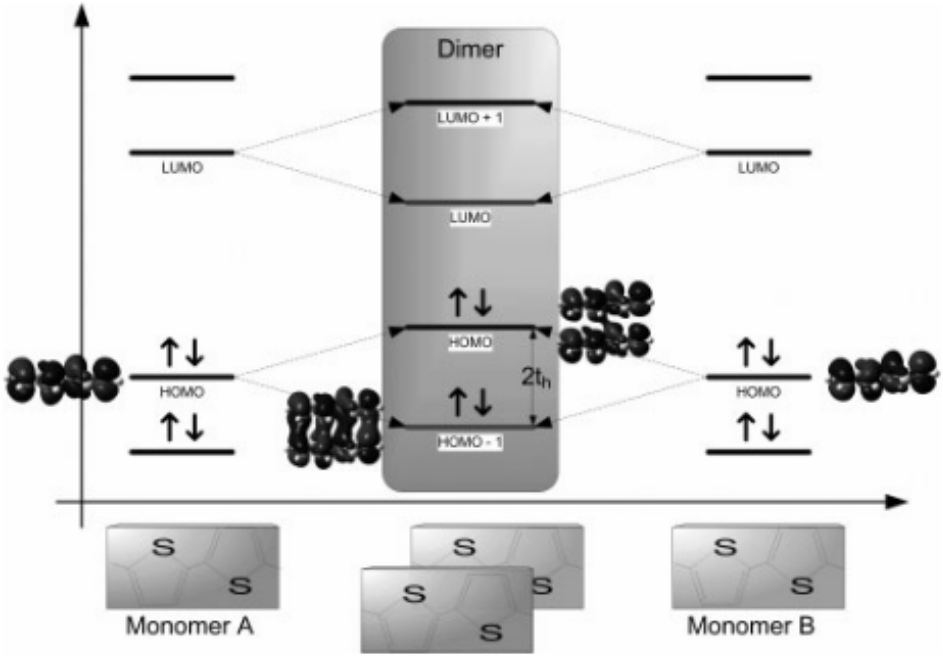


Figure 2: Splitting of the HOMO and HOMO-1 in the dimer

ESID method

Transfer integral for hole

$$t_{\text{hole}} = \frac{1}{2}\sqrt{(E_H - E_{H-1})^2 - (\varepsilon_1 - \varepsilon_2)^2}$$

$$t_{\text{hole}} = \frac{E_H - E_{H-1}}{2} \tag{1}$$

Tight-binding Hamiltonian

Relationship between charge-transport properties and geometric structure

$$H = \sum_{m} \epsilon_m a_m^+ a_m + \sum_{m \neq n} t_{mn} a_m^+ a_n$$

Research Methodology

pCCD based methods

- pCCD-LCCD/LCCSD
- fpCCSD/fpCCD
- IP-EOM-pCCD
- DIP-EOM-pCCD

PyBEST's support of molecular fragments...
Methods...

- Exact approach
- ESID method
- Approximate model

Testing...

Graphical user interface (GUI)

- A user-friendly graphical user interface...
- charge transport properties
- electron cross platform
- JavaScript Object Notation format
- Seprate Git-Lab repository.

Critical path and risk assessment

- Convergence-related difficulties in pCCD based calculations.

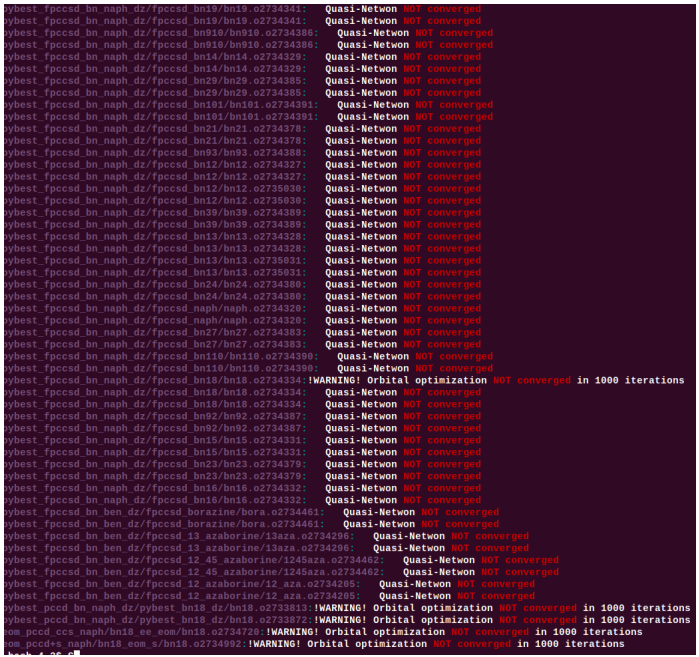


Fig-1 Quasi-Newton not converged

- Might have numerical difficulties (for instance, solving the amplitude equations for pCCD-LCCSD)
- Unreliable electronic structures.

DMRG code...

Application

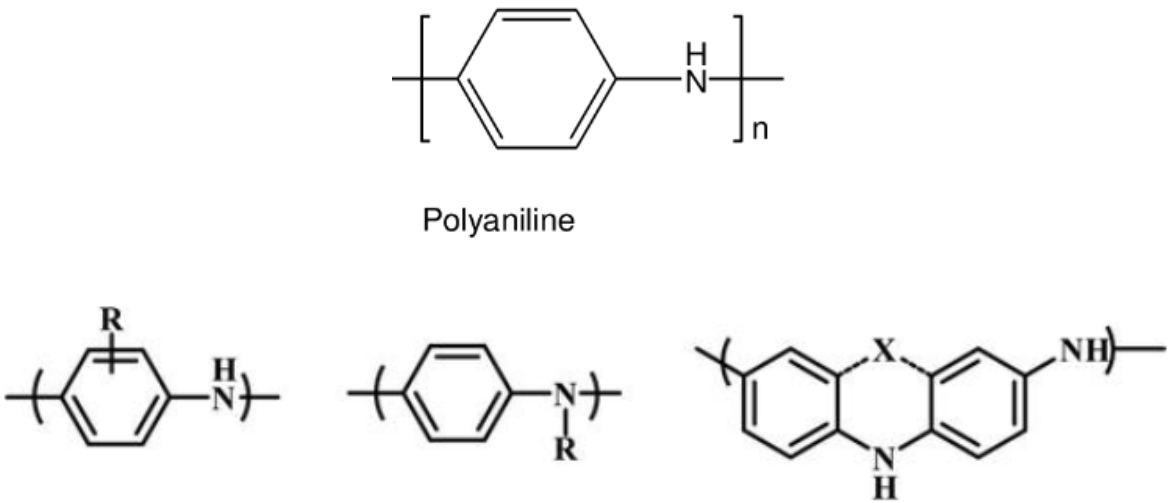


Figure 3: Polyaniline(Top) and its derivatives(Bottom)

Application

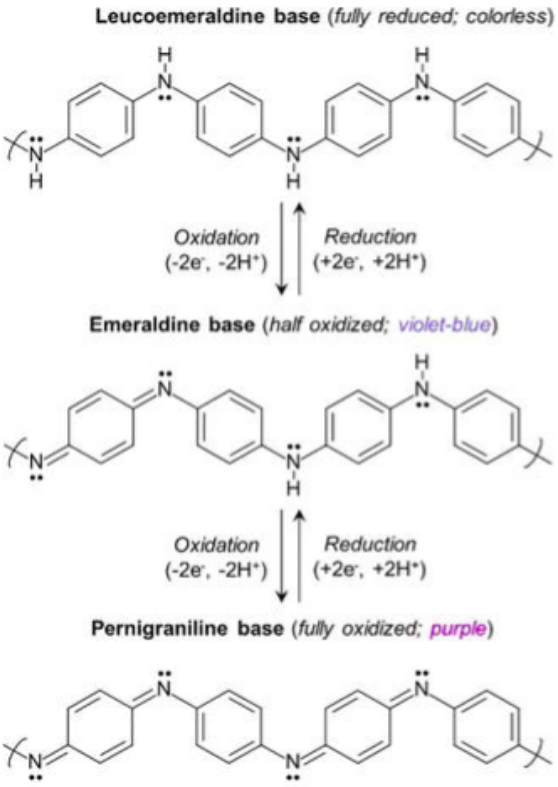


Figure 4: Polyaniline in its idealized oxidation states

Conclusion

Work package-A

- Charge transport module in PyBEST

Work package-B

- GUI for modeling charge transport properties

Work package-C

- Calculation of electronic structures and charge transport properties

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