

# Charge transport properties in organic electronics

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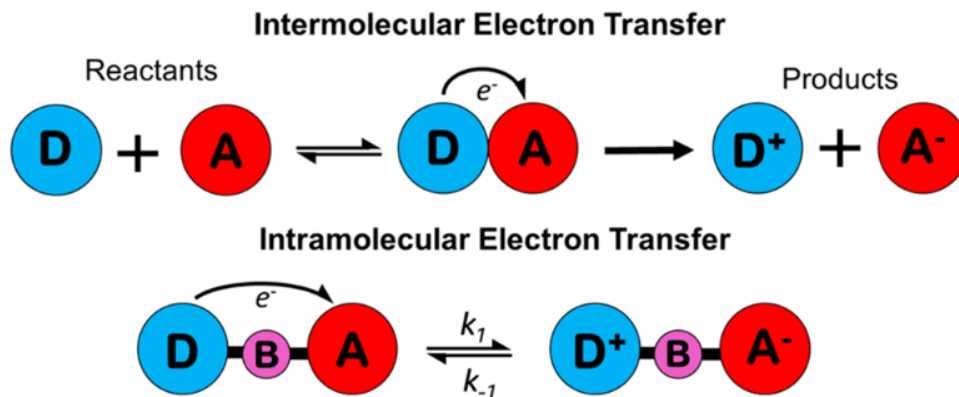
# Introduction

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

# Main objectives

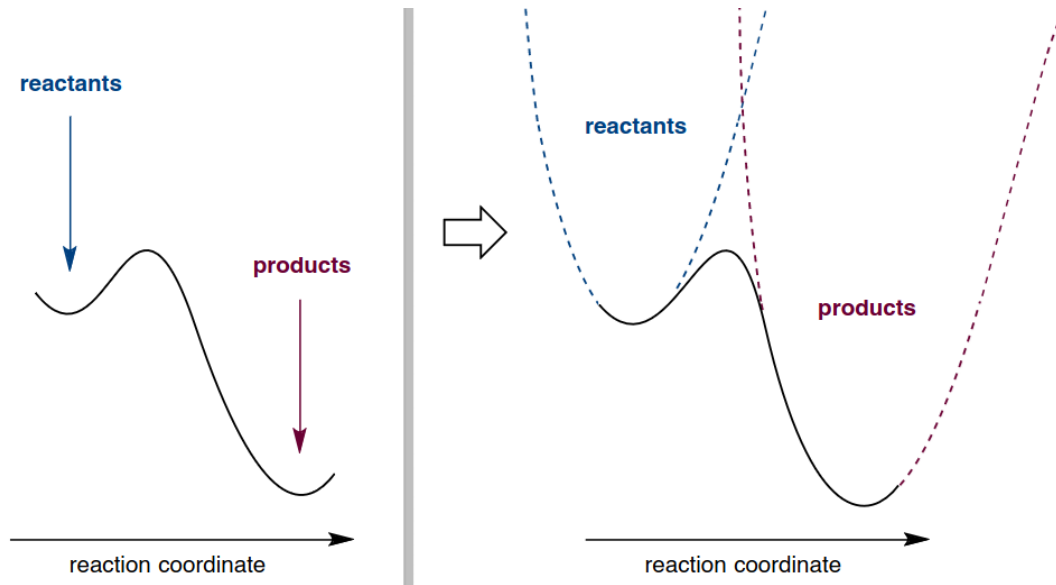
- The design, implementation, and testing of charge transfer models
- The design and implementation of a graphical user interface
- Quantum entanglement and correlation analysis

# Electron transfer

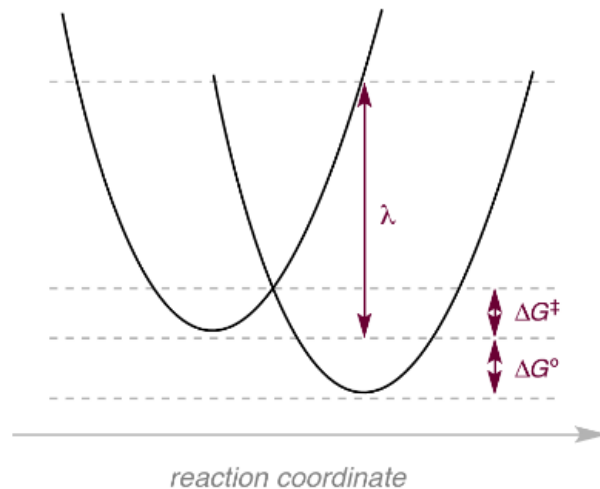
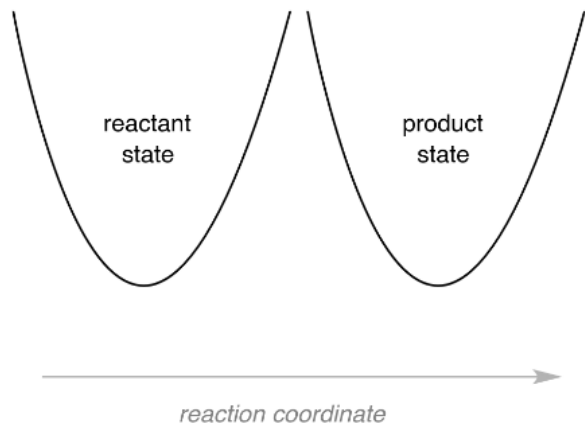


(Top): Formation of encounter complex  
(Bottom): Rigid molecular bridge

# Marcus theory

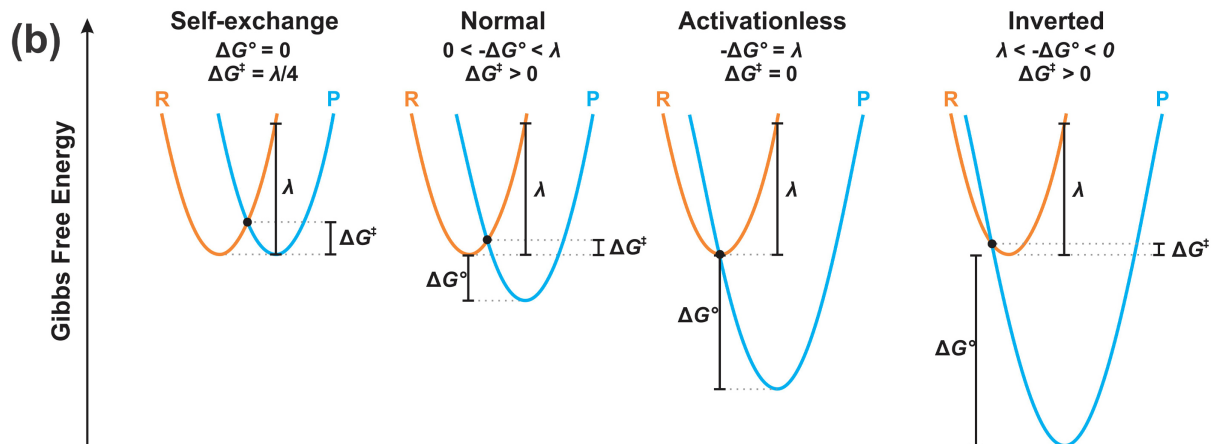
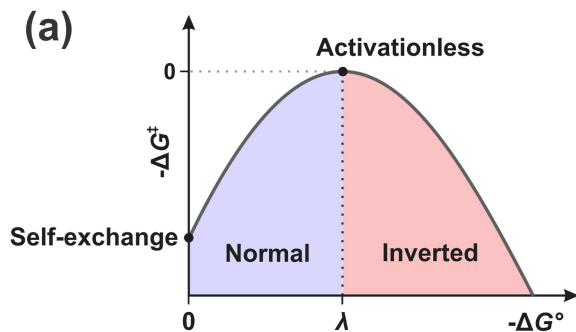


# Marcus theory



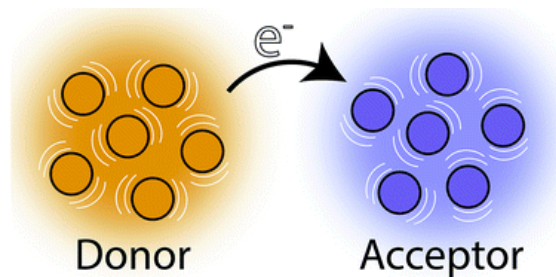
$$\Delta G^\ddagger = \frac{(\lambda + \Delta G^\circ)^2}{4\lambda}$$

# Marcus theory





# Marcus-theory



The electron transfer rate..

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

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

# Reorganization energy

The reorganization energy  $\lambda$  is defined as

$$\lambda = (E_{neutralgeometry}^{charged} - E_{neutralgeometry}^{neutral}) + (E_{chargedgeometry}^{neutral} - E_{chargedgeometry}^{charged})$$
$$\lambda = \lambda_1 + \lambda_2$$

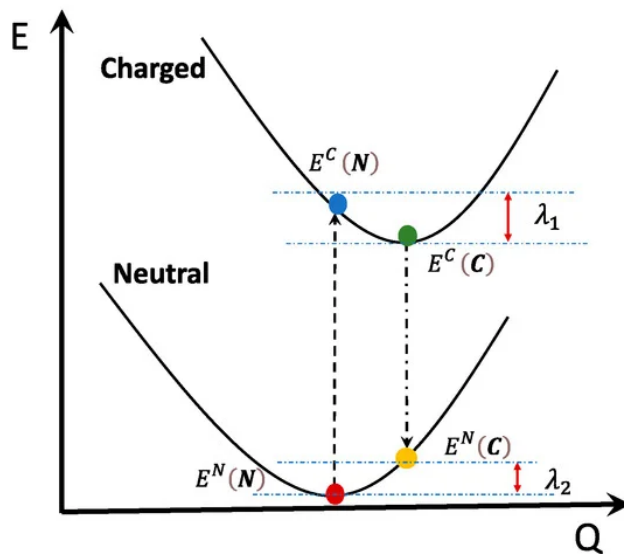


Figure 1: Adiabatic potential energy curves

# Charge transfer integral

$$V = \frac{J - S(e_1 + e_2)/2}{1 - S^2} \quad \text{---} > (a)$$

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

$$S = \langle \phi_1 | \phi_2 \rangle \quad \text{---} > (c)$$

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

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

# ESID Method

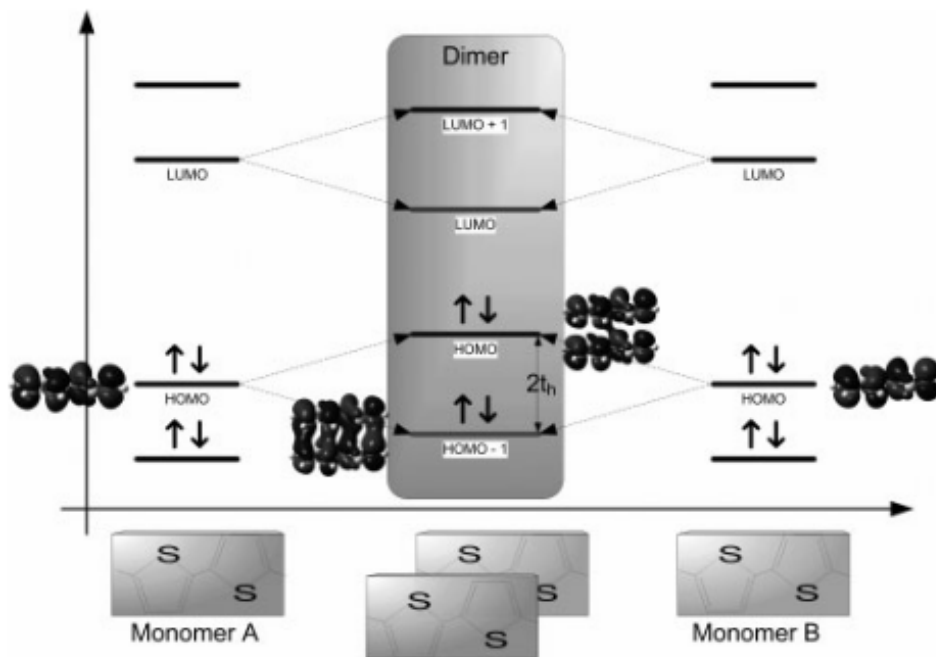


Figure 2: Splitting of the HOMO and HOMO-1 in the dimer

Transfer integral for hole

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

$$t_{\text{hole}} = \frac{E_H - E_{H-1}}{2} \quad (1)$$

# Tight-binding Hamiltonian

Relationship between charge-transport properties and geometric structure

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

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.

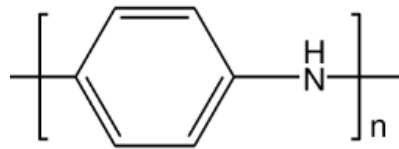
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```

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

DMRG code...

Fig-1 Quasi-Newton not converged

# Application



Polyaniline

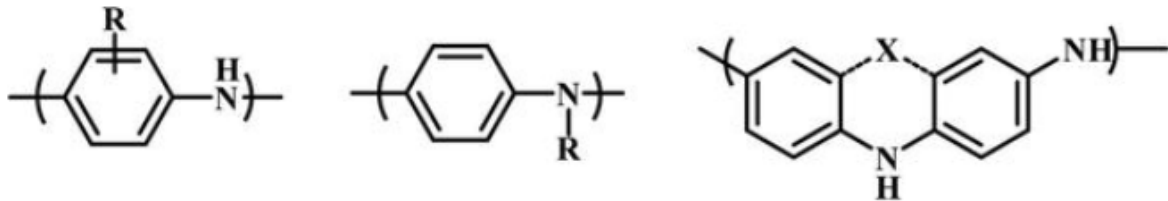


Figure 3: Polyaniline(Top) and its derivatives(Bottom)

# Application

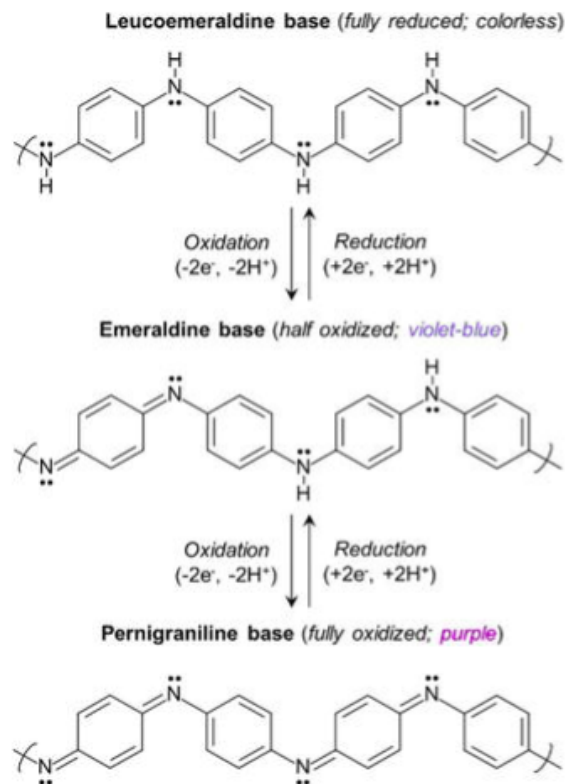


Figure 4: Polyaniline in its idealized oxidation states

# 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

# Acknowledgement

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