

ASCOTによる量子伝導解析

東京大学生産技術研究所

産学官連携研究員

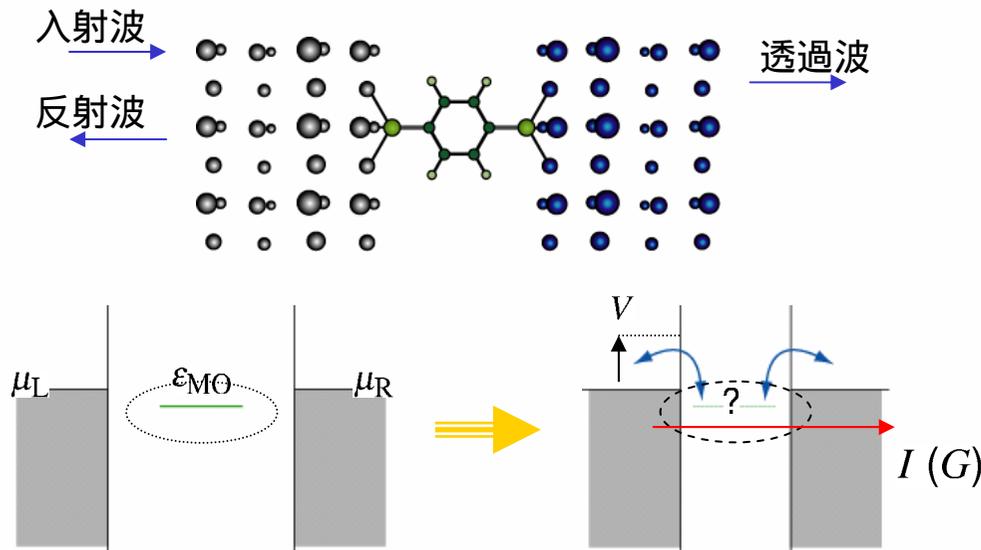
近藤 恒



対象となる系と新たな計算法(開放系)の必要性

ナノスケールのデバイスの可能性に関連

単分子等によるナノ構造体の示す伝導特性



全系の電子状態と伝導特性:

- 電極の構造
- ナノ構造体(分子)の構造
- コンタクトの構造

バイアス下での定常状態の計算 (I - V 曲線)



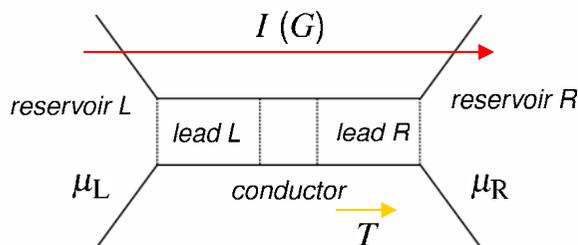
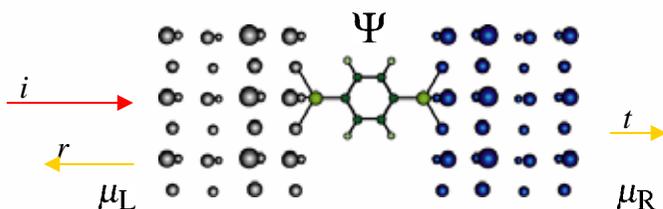
密度汎関数計算

境界条件	
周期系(結晶) ⇔	周期境界条件
孤立系(分子等) ⇔	無限遠でゼロ
開放系 ⇔	散乱状態の境界条件

非平衡グリーン関数法

計算手法

Landauer Formula



- Current I

$$I = \frac{2e}{h} T (\mu_L - \mu_R)$$

where

T : transmission coefficient

- Conductance G

$$G = \frac{I}{(\mu_L - \mu_R)/e} = \frac{2e^2}{h} T$$

Methods

- Wave function
 - ▶ Lippmann-Schwinger eq.
 - ▶ Overbridging Boundary Matching (OBM) method
- Green's Function
 - ▶ Non-Equilibrium Green's Function (NEGF) method

計算手法: 非平衡グリーン関数法

Band

Electrodes

- H_L : left region
- H_R : right region
- $V_H(r)$: left/right region

Junction

- H_C : central region
- $\rho(r)$: central region

boundary condition: periodic system

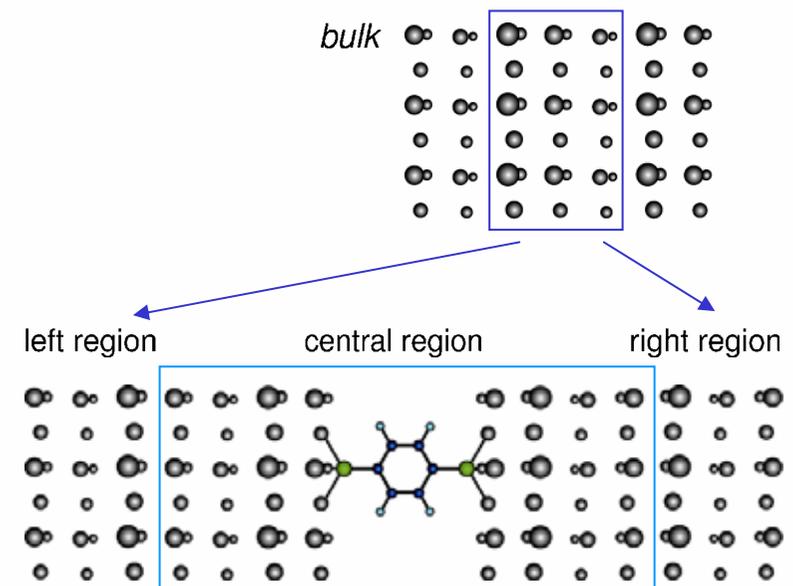
- Hamiltonian matrix

$$\mathcal{H} = \begin{pmatrix} H_L & H_{LC} & 0 \\ H_{CL} & H_C & H_{CR} \\ 0 & H_{RC} & H_R \end{pmatrix}$$

Electronic structure & Transport

- H_C : central region
- $\rho(r)$: central region
- $G_C(z) = [zS_C - H_C - \Sigma_R(z) - \Sigma_L(z)]^{-1}$
- $T(\epsilon) = \text{Tr} [\Gamma_L(\epsilon) G_C^r(\epsilon) \Gamma_R(\epsilon) G_C^a(\epsilon)]$
- $I = \frac{2e}{h} \int d\epsilon T(\epsilon) [f(\epsilon - \mu_L) - f(\epsilon - \mu_R)]$

boundary condition: open system



電荷密度の計算法

$$\circ \rho_C = \frac{1}{2\pi i} \int_{-\infty}^{\infty} d\varepsilon G_C^<(\varepsilon)$$

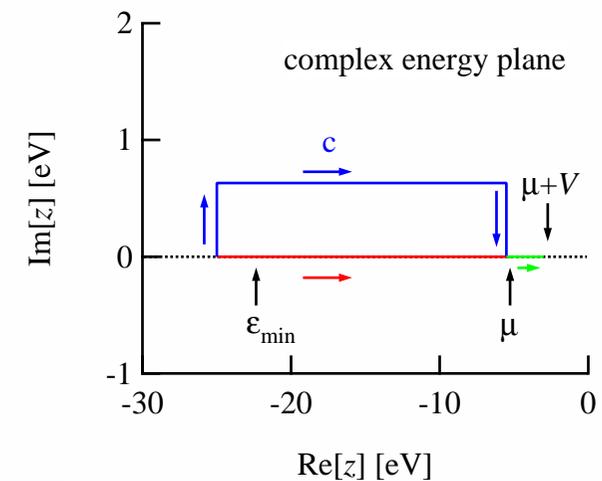
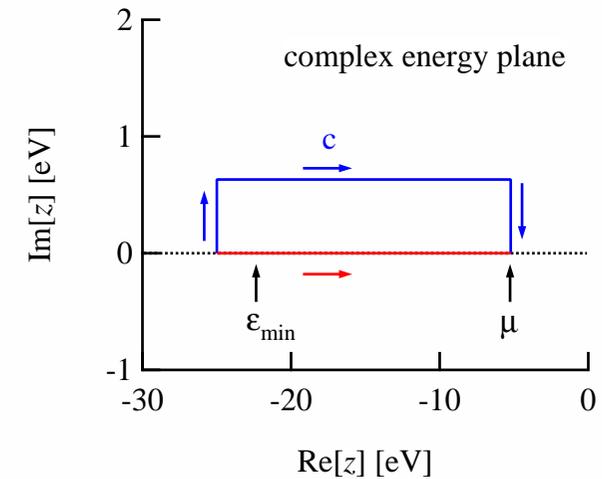
$$\bullet V = 0.0[\text{V}]$$

$$\begin{aligned} \rho_C &= -\frac{1}{\pi} \text{Im} \int_{-\infty}^{\mu} d\varepsilon G_C^r(\varepsilon) \\ &= -\frac{1}{\pi} \text{Im} \int_c dz G_C^r(z) \end{aligned}$$

$$\bullet V \neq 0.0[\text{V}]$$

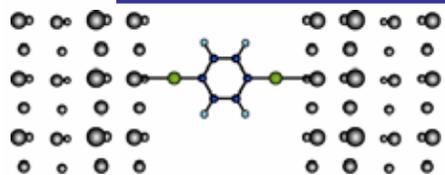
$$\begin{aligned} \rho_C &= -\frac{1}{\pi} \text{Im} \int_{-\infty}^{\mu} d\varepsilon G_C^r(\varepsilon) + \frac{1}{2\pi i} \int_{\mu}^{\infty} d\varepsilon G_C^<(\varepsilon) \\ &= -\frac{1}{\pi} \text{Im} \int_c dz G_C^r(z) + \frac{1}{2\pi i} \int_{\mu}^{\infty} d\varepsilon G_C^<(\varepsilon) \end{aligned}$$

$$G_C^<(\varepsilon) = G_C^r(\varepsilon) i(\Gamma_L(\varepsilon) f(\varepsilon - \mu_L) + \Gamma_R(\varepsilon) f(\varepsilon - \mu_R)) G_C^a(\varepsilon)$$



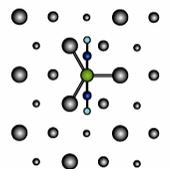
計算例: ベンゼンジチオール分子1

Kondo *et al.*:
PRB **73** (2006) 235323.

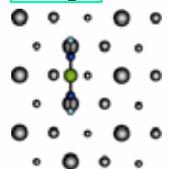


Contact structure

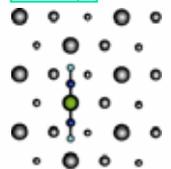
Hollow



Bridge

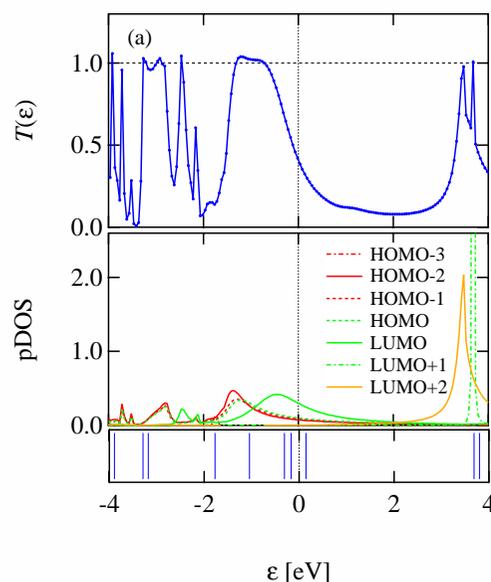


Ontop



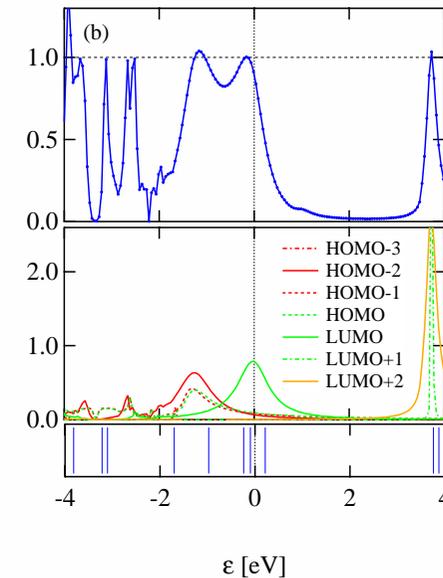
Hollow

$T(\epsilon_F) \sim 0.4$



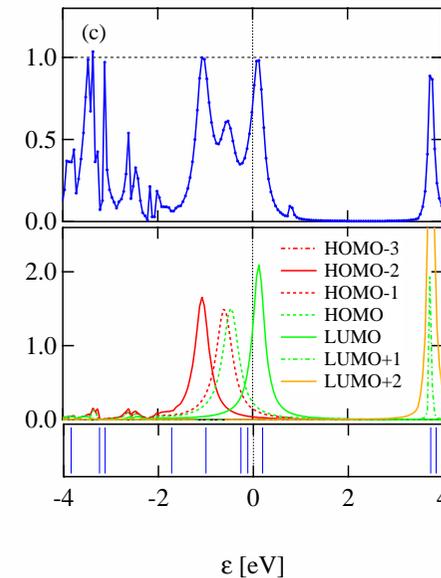
Bridge

$T(\epsilon_F) \sim 0.9$

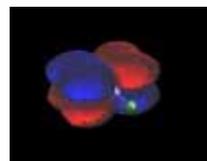


Ontop

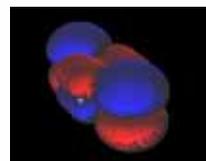
$T(\epsilon_F) \sim 0.8$



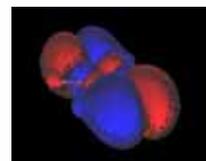
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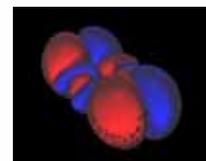
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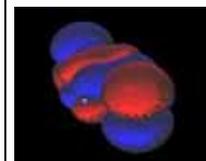
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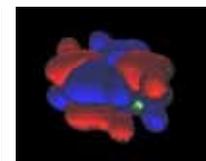
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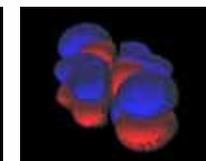
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分子軌道の広がり

・結合の強さに依存

・分子軌道の対称性による

➤ Experimental work

Brak junction technique

$$G = 10^{-4} G_0$$

[Reed *et al.*: Science **278** (1997) 252.]

STM

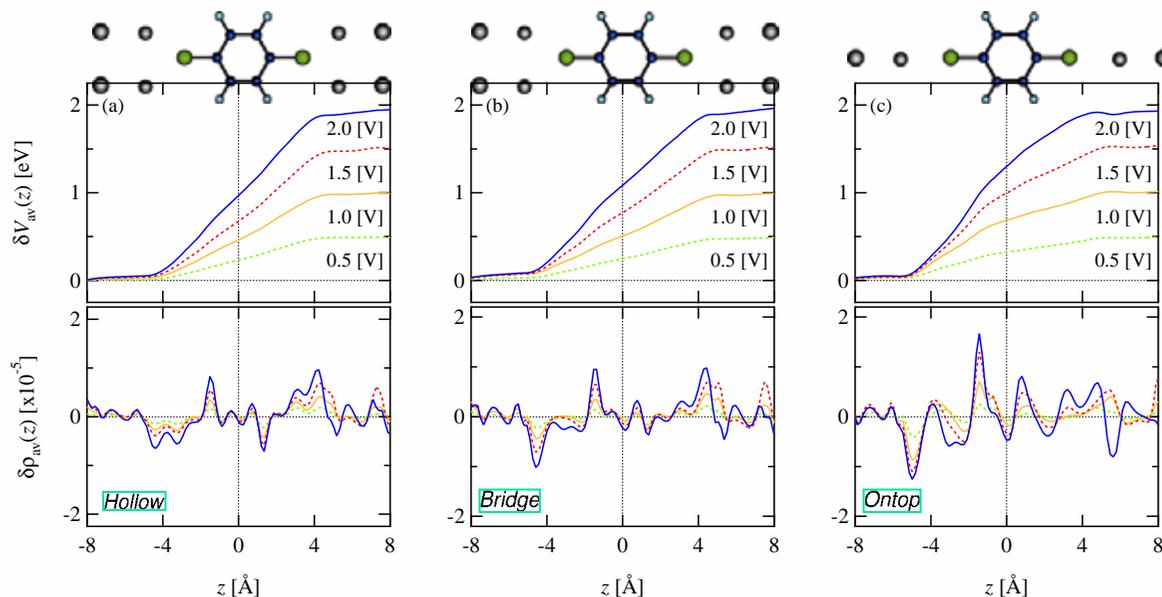
$$G = 0.011 G_0$$

[Xiao *et al.*: Nano Lett. **4** (2004) 267.]

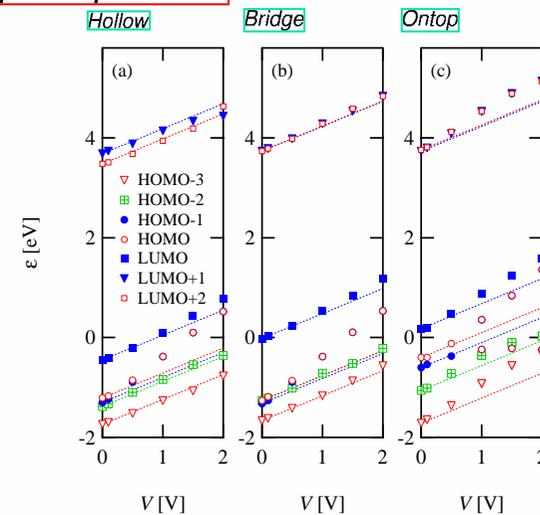
計算例：ベンゼンジチオール分子2

Kondo *et al.*:
PRB **73** (2006) 235323.

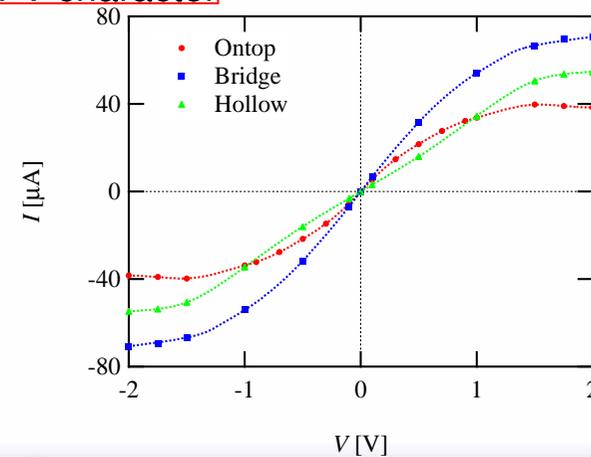
potential drop



peak position

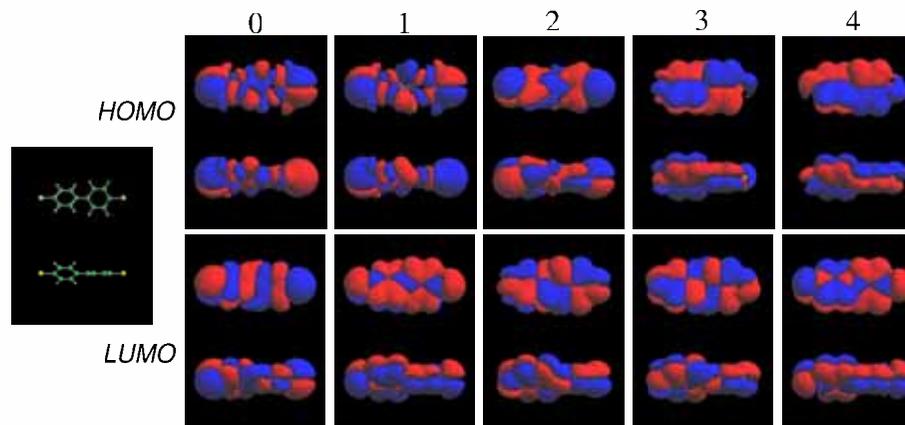
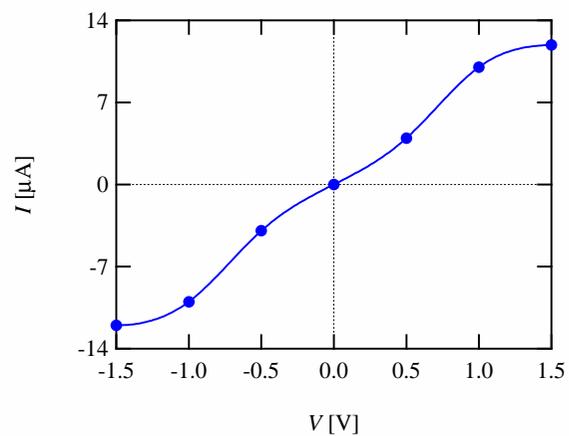
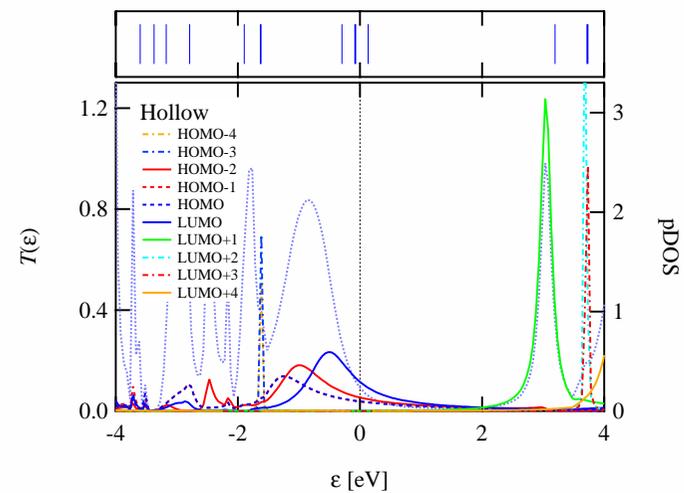
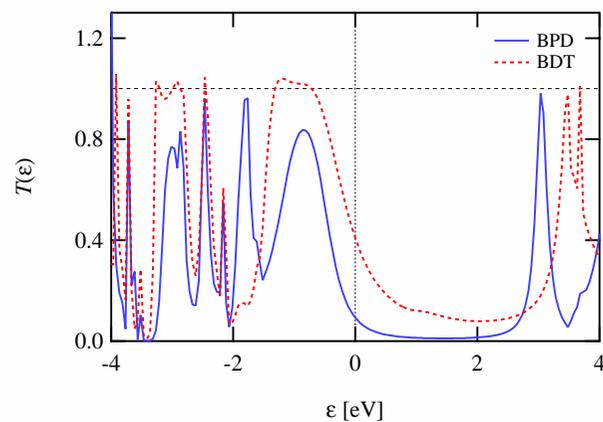
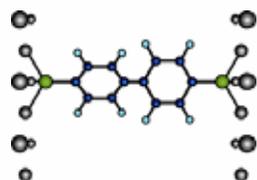


I-V character



- ✓ 分子と電極との間の結合が弱いOntopの時、unusualな振る舞いが見られる。
- ✓ 適当な結合の大きさのBridgeで最大の電流値を得た。

計算例: ビフェニルジチオール分子

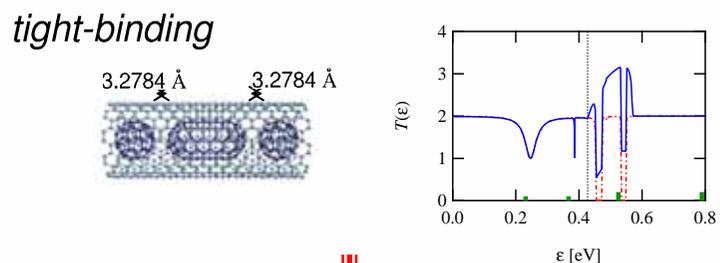


プログラムの公開

Computer Software for Transport-property Analysis (ASCOT)

<http://www.fsis.iis.u-tokyo.ac.jp/result/software/>, June 2005.

文部科学省ITプログラム「戦略的基盤ソフトウェアの開発」



DFT版: 12月公開予定

文部科学省次世代IT基盤構築のための研究開発
 「革新的シミュレーションソフトウェアの研究開発」

