



Univ Tsukuba



ナノスケール系の量子伝導シミュレーション

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原子分子レベルからの電子状態研究

computational material science
nano simulation
computational nanotechnology

基礎物理
固体物理学
ナノサイエンス
物質科学
ナノ構造の基礎物性

ナノテクノロジーへの
応用研究
ナノエレクトロニクス
分子エレクトロニクス

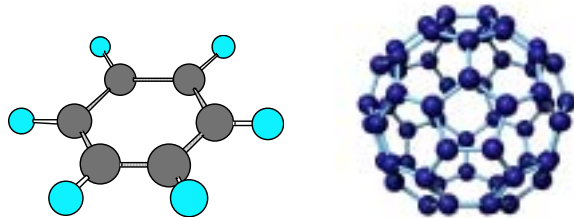
計算物性物理学
計算科学・シミュレーション研究
電子状態計算理論
大規模数値計算

ナノスケール系の電気伝導の理論シミュレーション

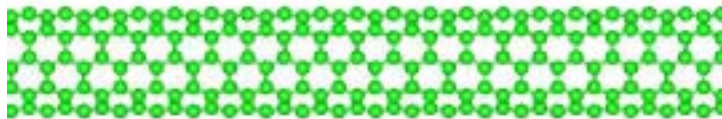
ナノスケール系

電気伝導

nm (ナノメートル)
 10^{-9}



単一分子



カーボンナノチューブ

マクロ系

粒子性

オームの法則

$$V(\text{電圧}) = I(\text{電流}) \times R(\text{抵抗})$$



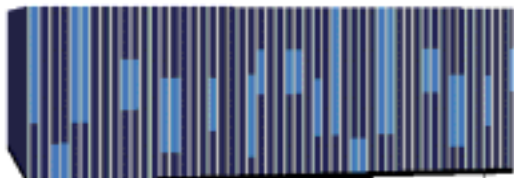
ナノスケール系

波動性

量子論に基づいた理論による
電気伝導特性解析

量子効果

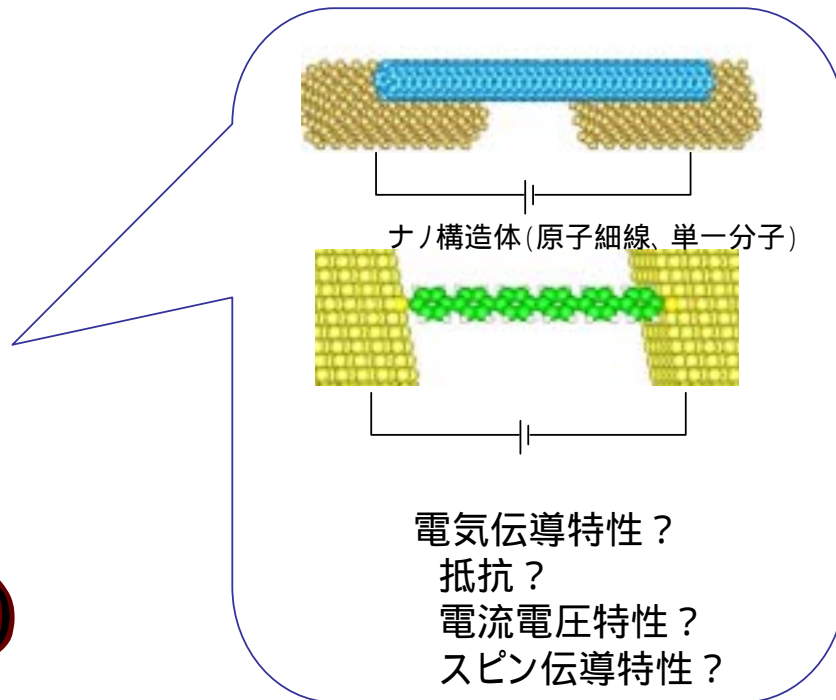
ナノスケール系の電子状態・電気伝導の理論シミュレーション



スーパーコンピュータシステム



PC Cluster

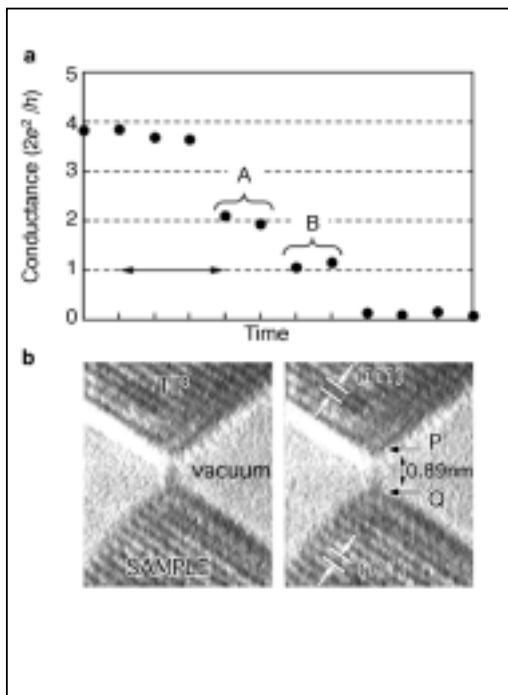


ナノスケールトランジスタ
ナノスケール配線
ナノスケールスイッチ

理論設計

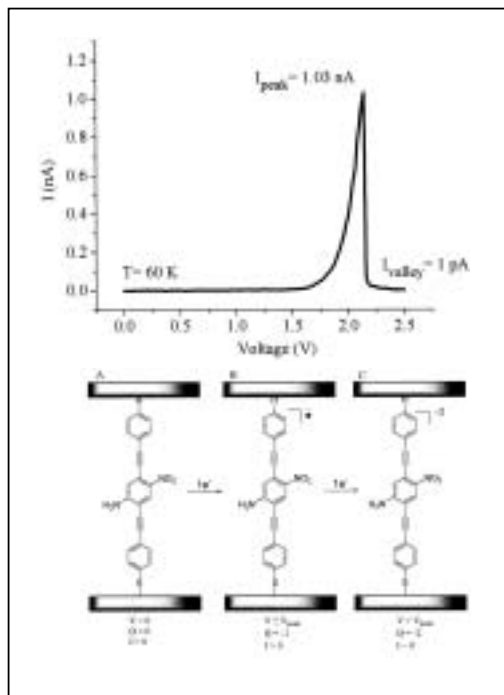
Experiments : Transport in nanostructures

Atomic wire



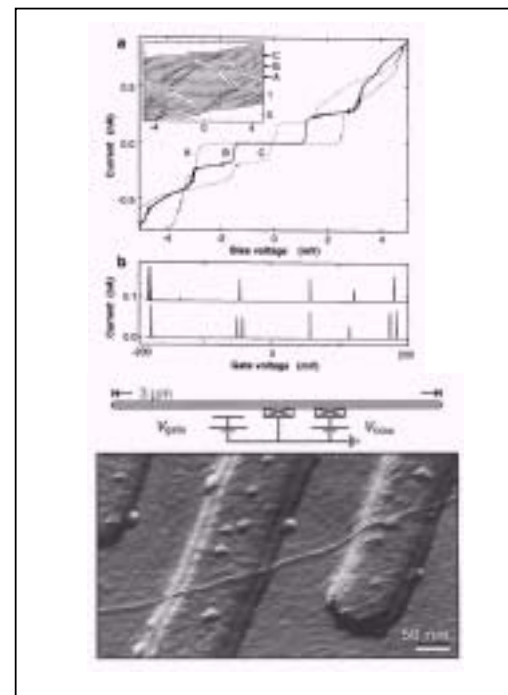
H. Ohnishi, Y. Kondo, K. Takayanagi,
Nature 395 780 (1998)

Molecule



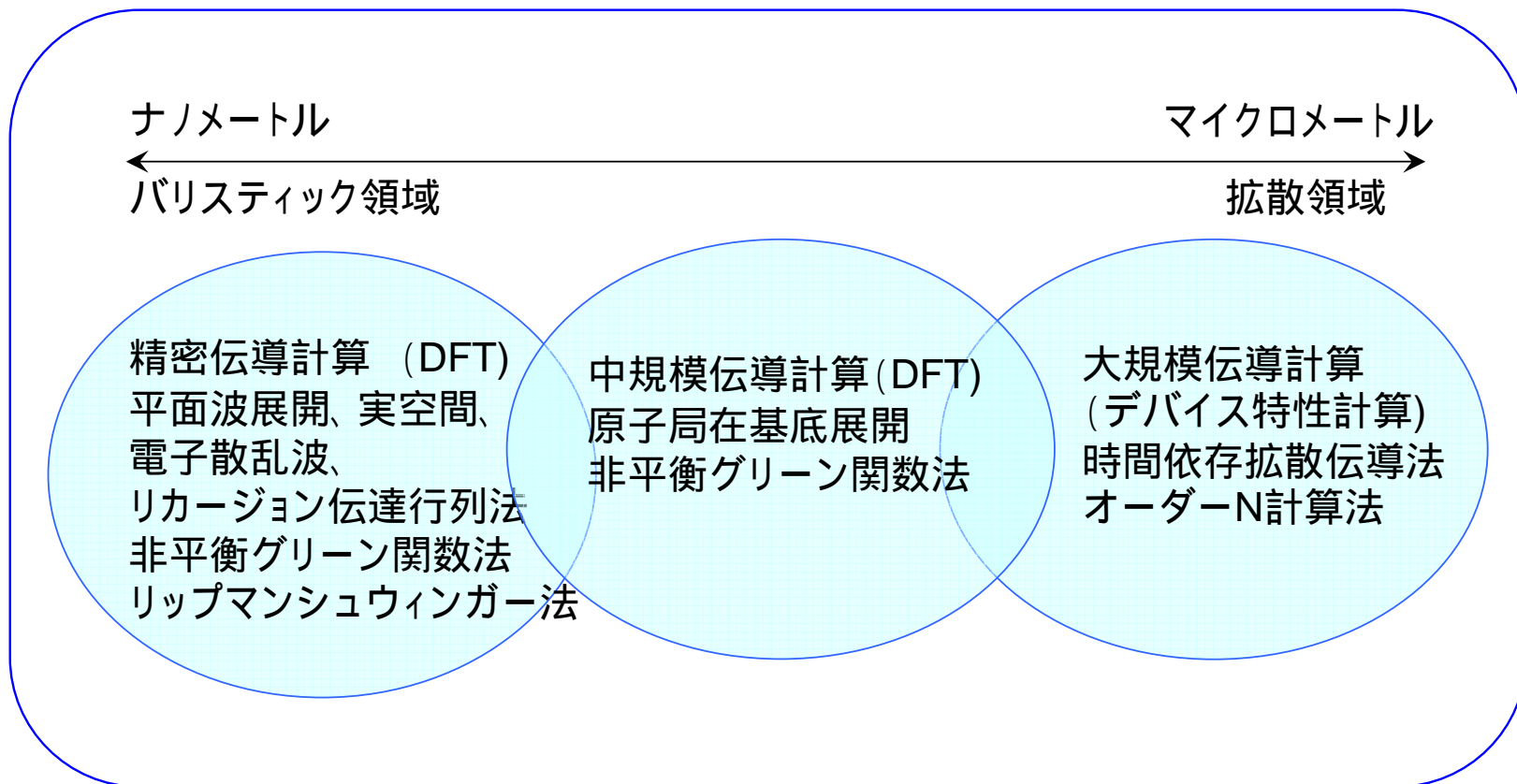
J. Chen, M. A. Reed, A. M. Rawlett,
J. M. Tour, Science 286 (1999) 1550

Nanotube

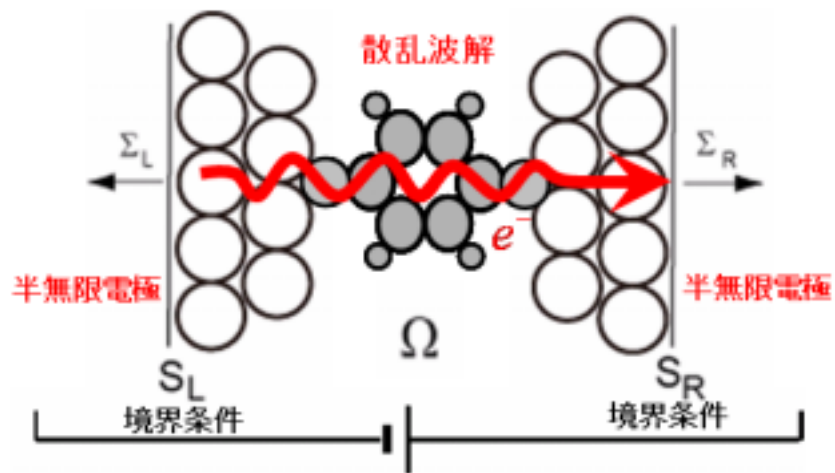
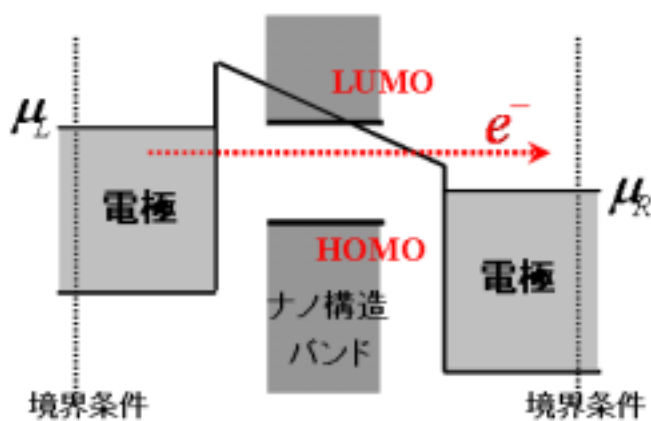


S. J. Tans, M. H. Devoret, H. Dai, A. Thess,
R. E. Smalley, L. J. Geerligs, C. Dekker,
Nature 386 (1997) 474

原子分子レベルからのマルチスケール量子伝導シミュレーション

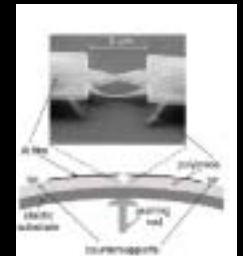
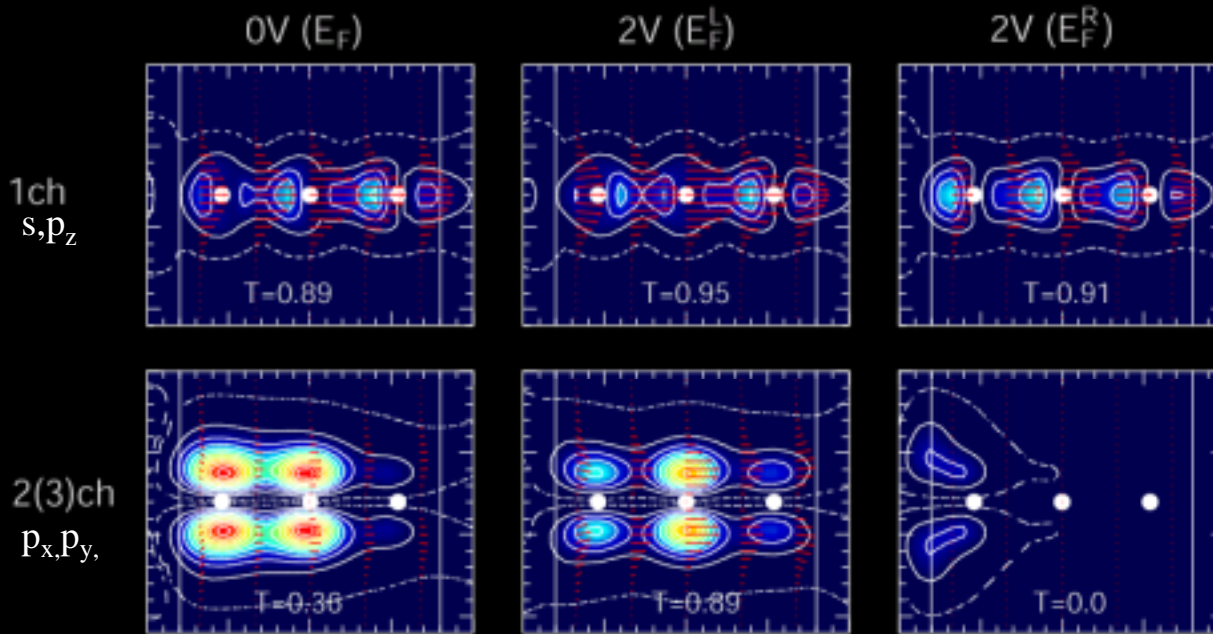
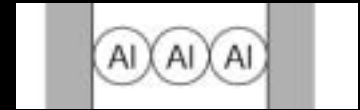


非平衡開放系の第一原理伝導計算

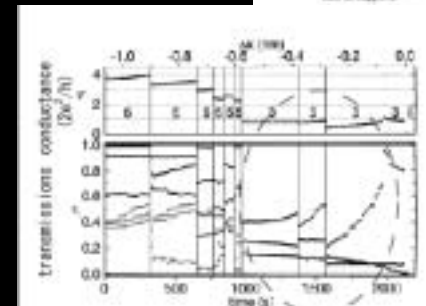
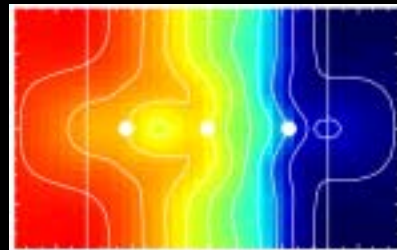


First-Principles Quantum Transport Calculation with Lippmann-Schwinger Equation

LDOS and current density distributions of Al atom wires

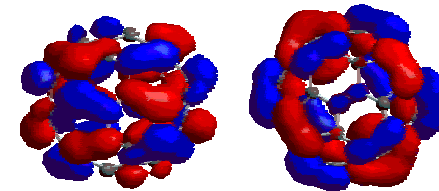
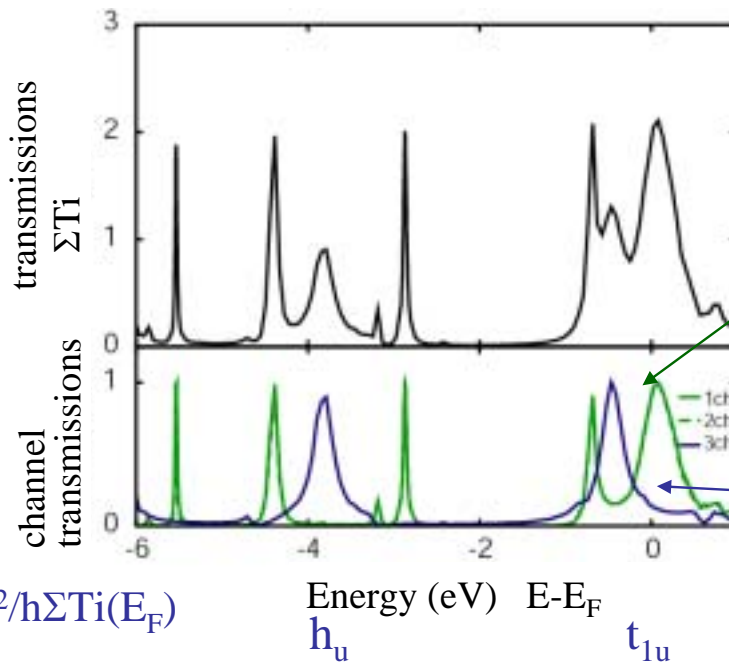


Potential drop 2V

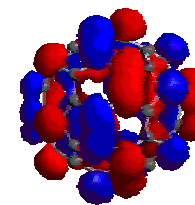


First-Principles Quantum Transport Calculation

Non-Equilibrium Green's Function Method with Localized Basis Set



LUMO 1ch LUMO 2ch



LUMO 3ch

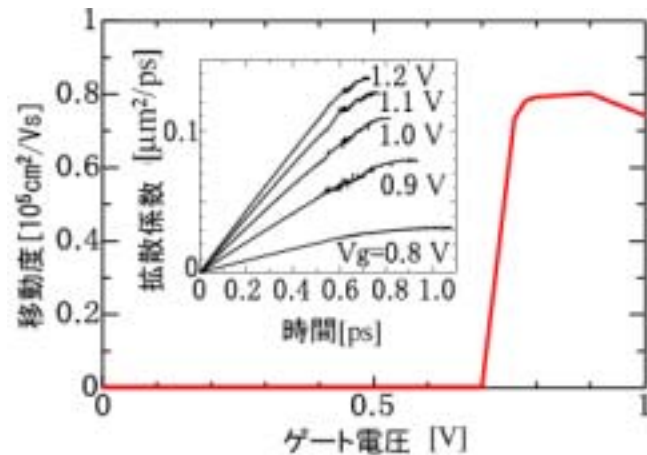
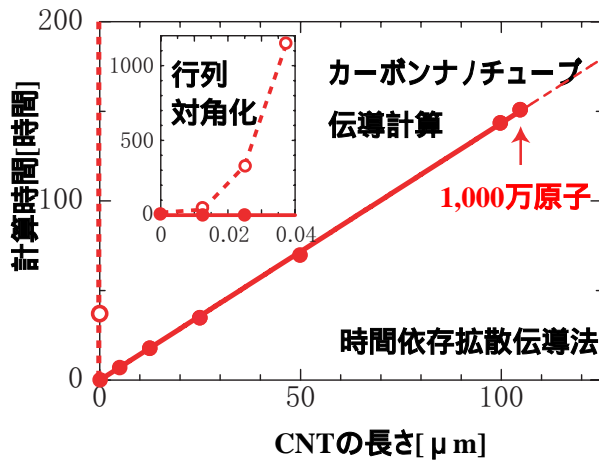
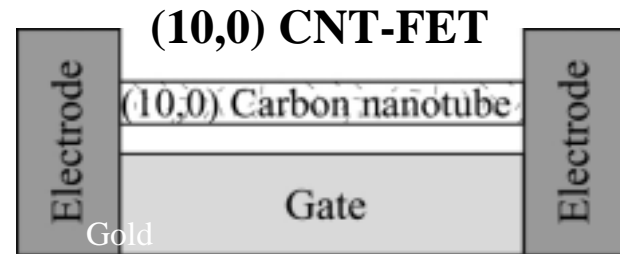
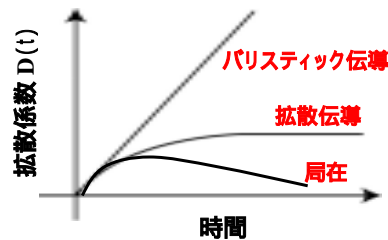
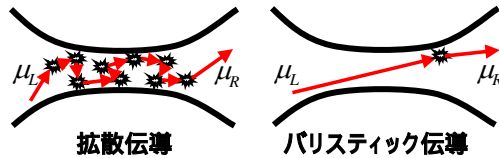
electron transfer from electrodes to C60
electron transport through LUMOs

$$G = 2e^2/h \Sigma T_i(E_F)$$

$$\text{Energy (eV) } E - E_F$$

N.Kobayashi, T.Ozaki, K.Tagami, M.Tsukada, K.Hirose, Jpn.J.Appl.Phys 45 2151 (2006)c

Time-Dependent Wave-Packet Diffusion Method CNT Field Effect Transistor (FET)



H.Ishii, N.Kobayashi, K.Hirose, PRB76 205432 (2007); Appl. Phys. Express 1 123002 (2008)

First-Principles Quantum Transport Calculation with Lippmann-Schwinger Equation

Density Functional Theory (DFT)

Local density approximation (LDA)

Lippmann-Schwinger Equation

$$\Psi(r) = \Psi^0(r) + \int dr' dr'' G(r, r') V(r', r'') \Psi(r'')$$

Laue representation

$$\Psi_n(r_{||}, z_p) = \exp(ik_{||} \cdot r_{||}) \sum \exp(iG_{||}^m \cdot r_{||}) \psi_m(iG_{||}^m \cdot z_p)$$

Probability current density^m

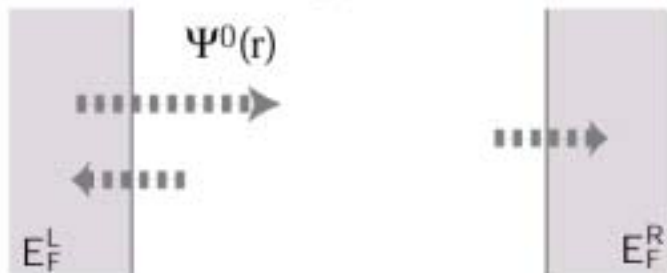
$$I(r) = \frac{2}{(2\pi)^3} \int dk \operatorname{Im} \Psi^*(r) \nabla \Psi(r)$$

Norm-conserving nonlocal pseudopotential

N.Kobayashi, M.Aono, M.Tsukada, PRB 64 121402R (2001)

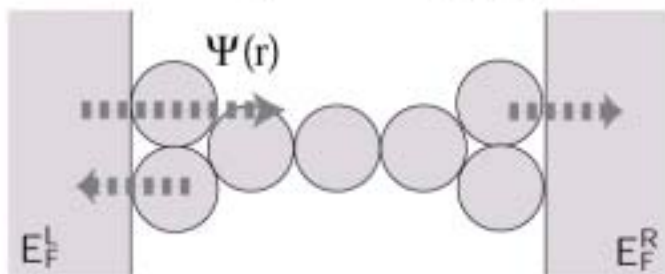
First-Principles Quantum Transport Calculation with Lippmann-Schwinger Equation

bimetallic electrode system H^0



$$(E - H^0)G(r, r') = \delta(r - r')$$

atom/molecule system $H = H^0 + V$



Lippmann-Schwinger equation

$$\Psi(r) = \Psi^0(r) + \int dr' dr'' G(r, r') V(r', r'') \Psi(r'')$$



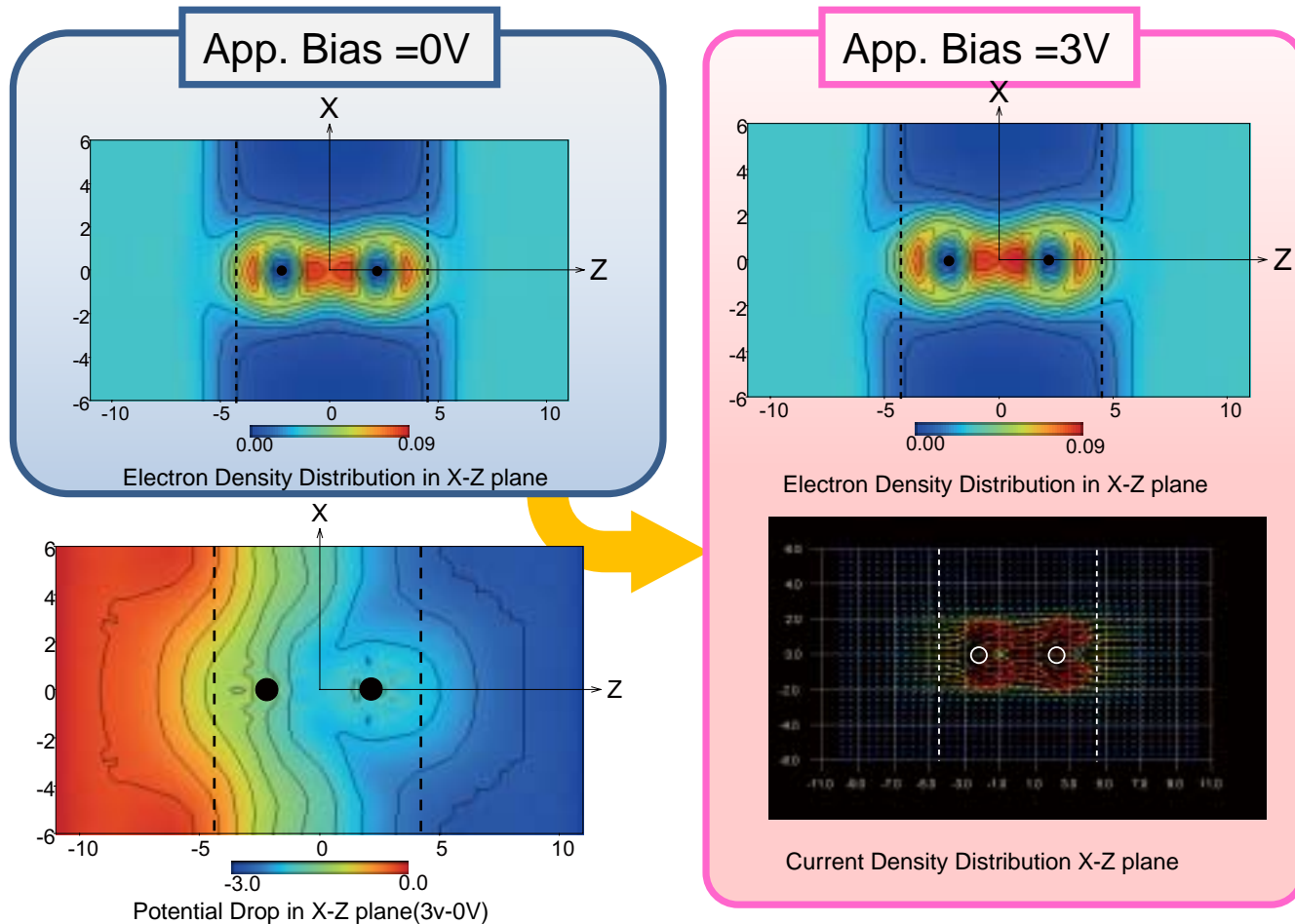
matrix Eq. $\underline{C} \underline{\Psi} = \underline{\Psi}^0$

Basis: 2D plane waves 1D real mesh

N.Kobayashi, M.Aono, M.Tsukada, PRB 64 121402R (2001)

Quantum Transport in Si Atom Wire

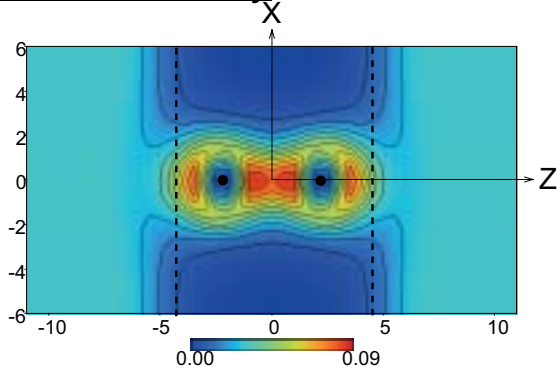
Effective Potential, Electron Density and Current Density



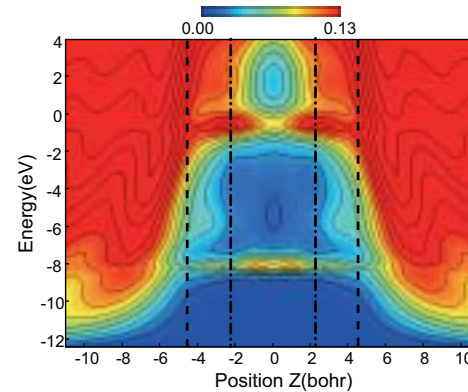
H.Kusaka, N.Kobayashi, J. Vac. Sci. Technol. B 27 (2009) 810

Quantum Transport in Si Atom Wire

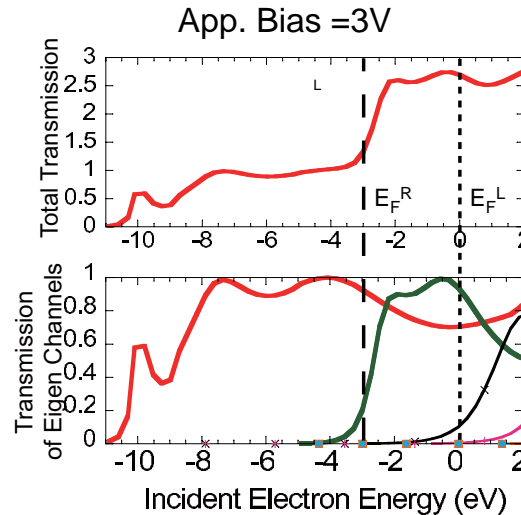
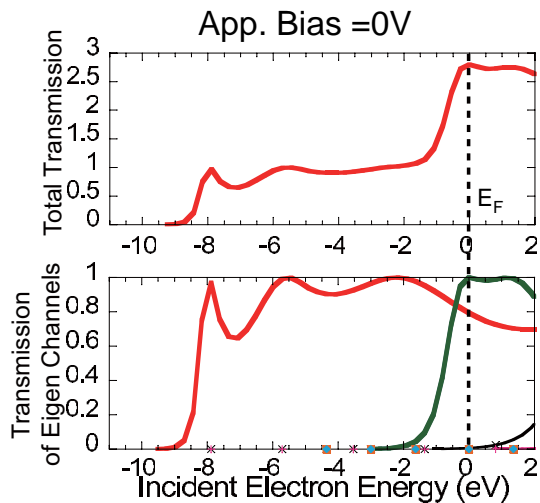
Electron Density



Local Density of States



Eigen Channels and Conductance

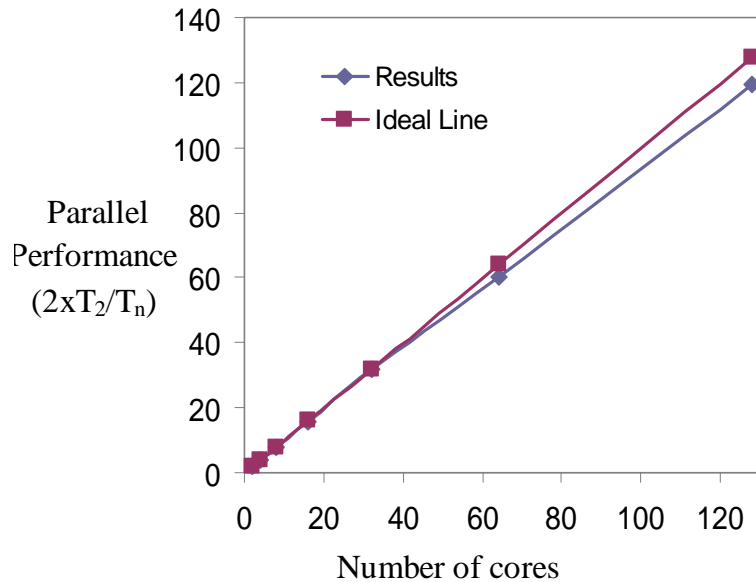


Three channels contribute to transport in Si atom wire.

H.Kusaka, N.Kobayashi, E-J. Surf.Sci. Nanotech 7 (2009) 17

Parallel Computing on PACS-CS, T2K

PACS-CS



T2K

