Currentdensity and eigenchannel: Implementation and application

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Corroborator

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STM experiment of eigenchannel on Pb(111) surface

Takeo Kato:

Eigenchannel analysis on Pb(111) surface

Taisuke Ozaki:

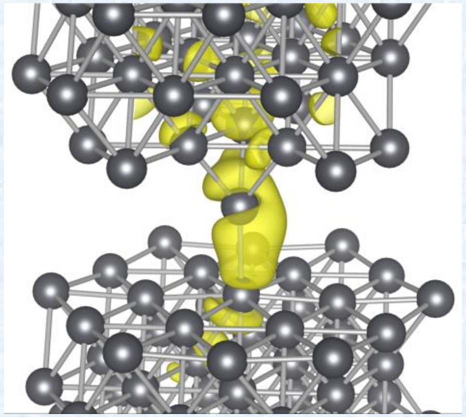
Currentdensity and eigenchannel

2016/11/25

2nd OpenMX developer's meeting

KAIST

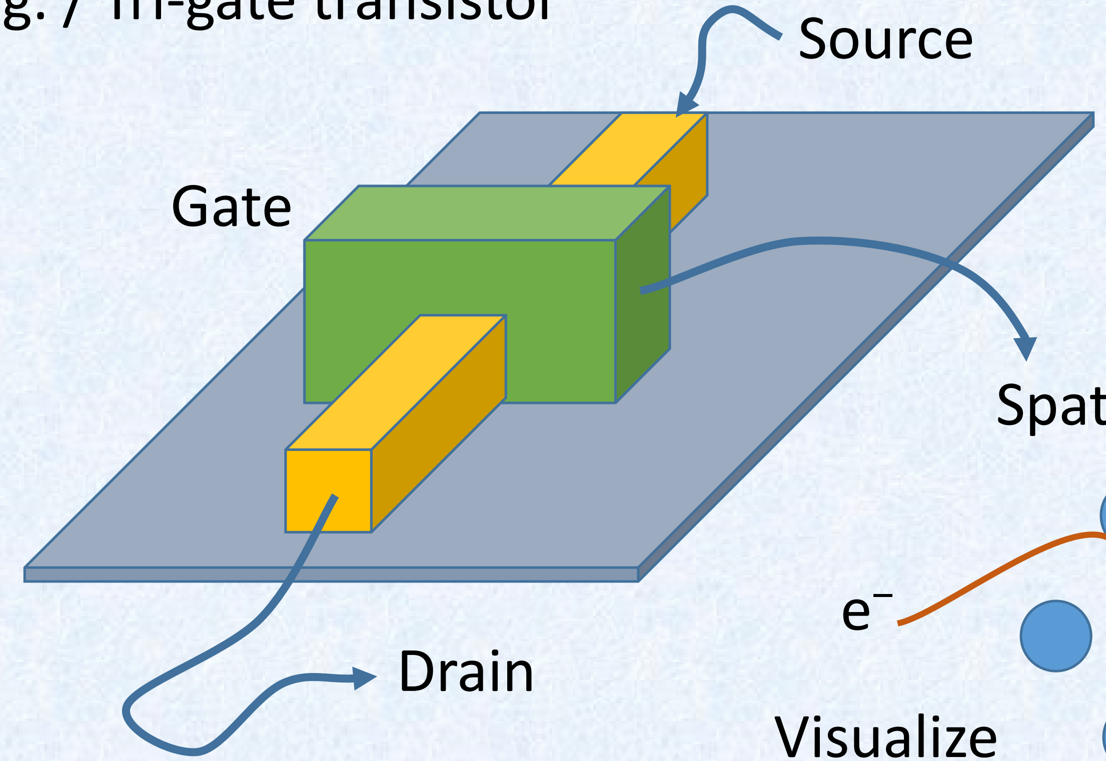
Outline



- Why eigenchannel and currentdensity ?
- Part 1. Eigenchannel on Pb(111) surface
  - Motivation: STM experiment of Pb(111) surface
  - First-principles eigenchannel analysis
  - Result
  - Summary
- Part 2. Implementation of currentdensity in OpenMX
  - Motivation
    - Conventional method for currentdensity
  - Method
    - Currentdensity in NEGF method
    - Difficulty and improvement
  - Result
    - 8−Zigzag Graphene Nanoribbon with domain wall
  - Summary

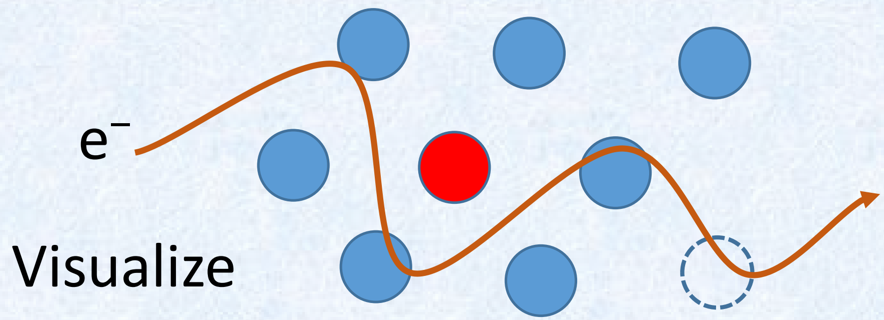
Motivation

E.g. / Tri-gate transistor



- Transmission
- Total current
- Conductance

Spatial information



Real-space picture for the conducting phenomena in a nano device

OpenMX and Software Advancement project@ISSP

- Eigenchannels
- Real-space current density

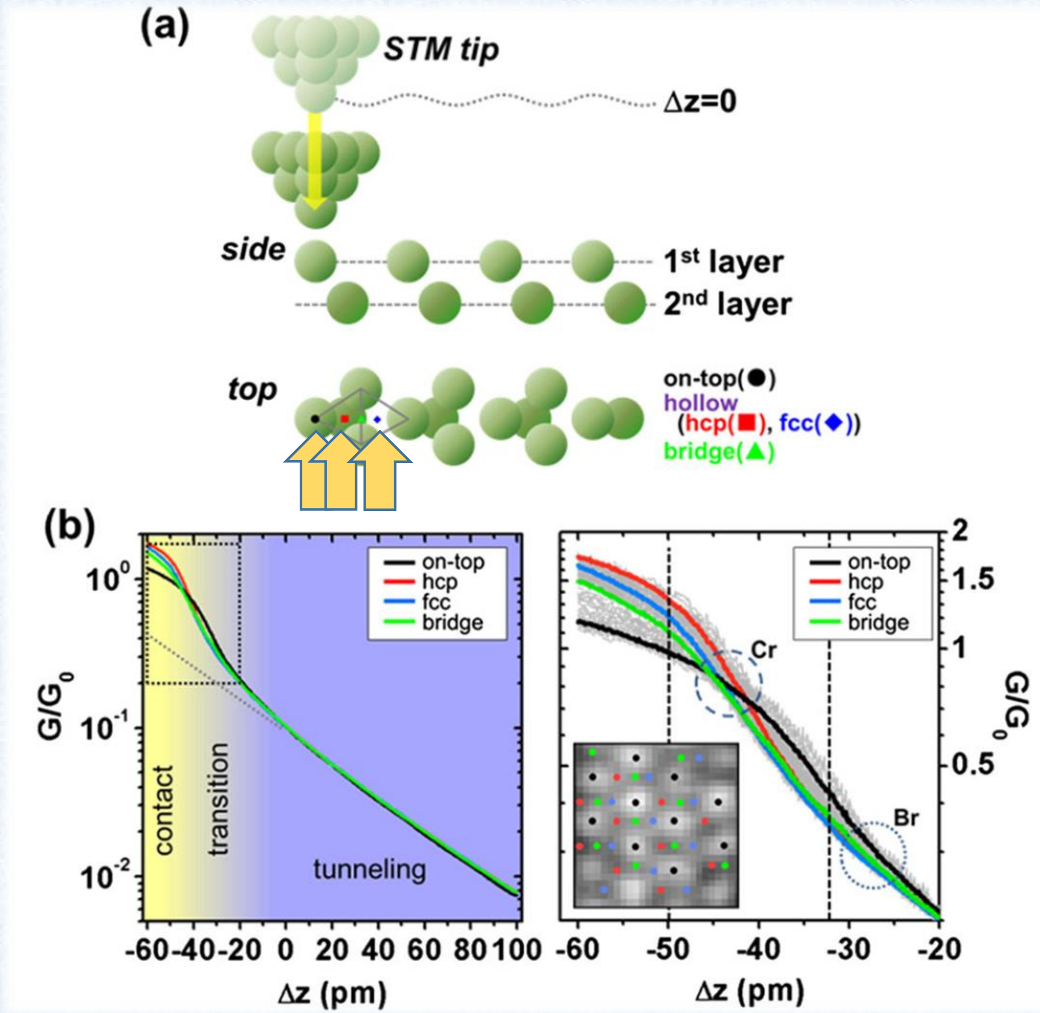
Conductance evolution and tip position

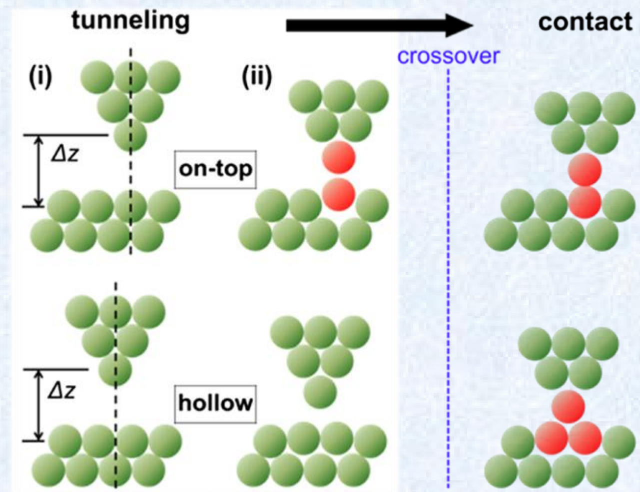
H. Kim and Y. Hasegawa, PRL 114, 206801 (2015).

On-top: The first-layer Pb atom lies just under the tip.

hcp: The second-layer Pb atom lies just under the tip. 3 nearest neighbor atoms on the surface.

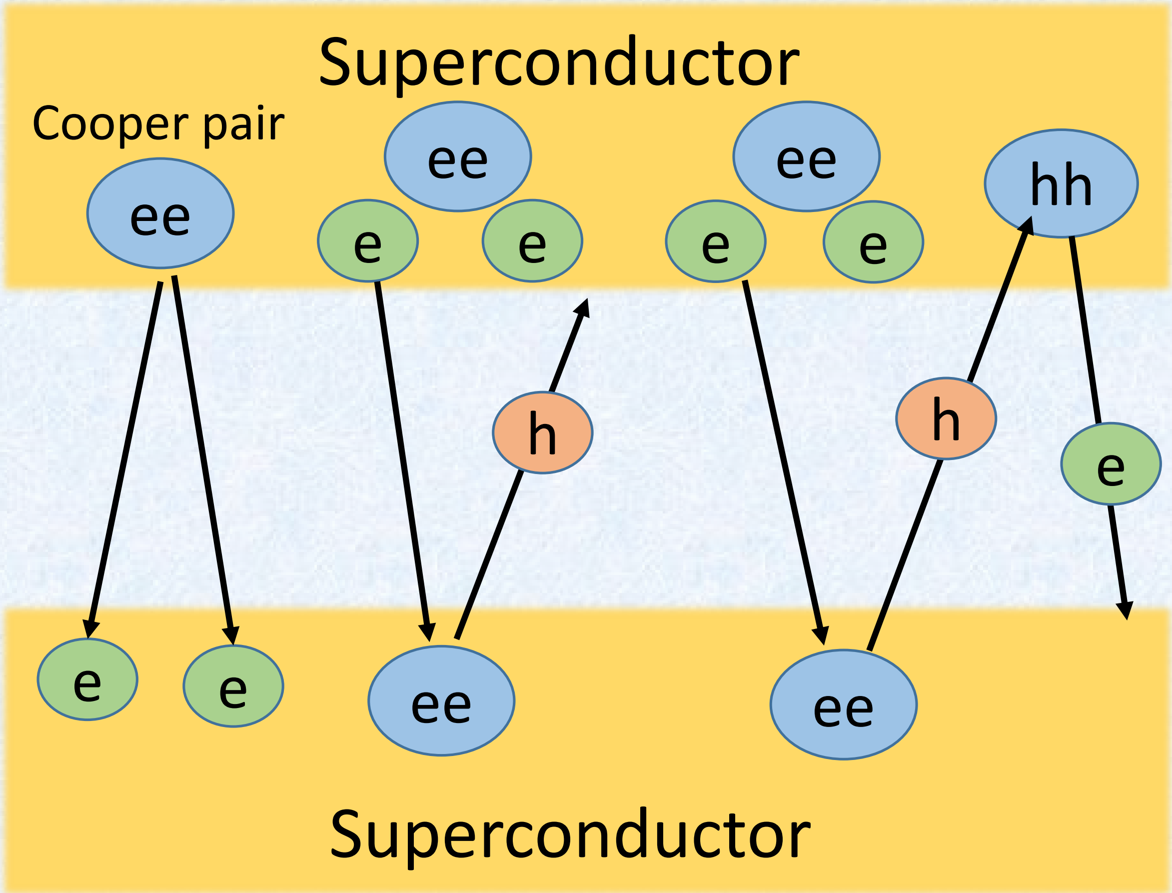
fcc: The third-layer Pb atom lies just under the tip.



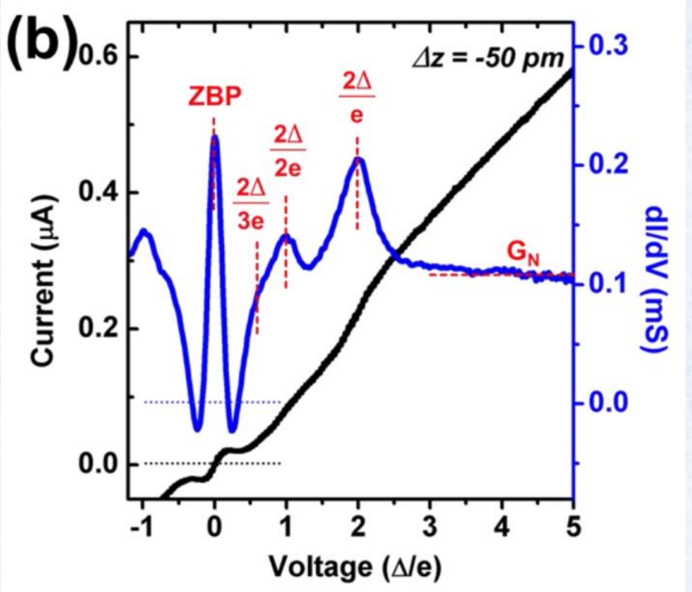


Eigenchannel in the STM experiment

H. Kim and Y. Hasegawa, arXiv: 1506.05528

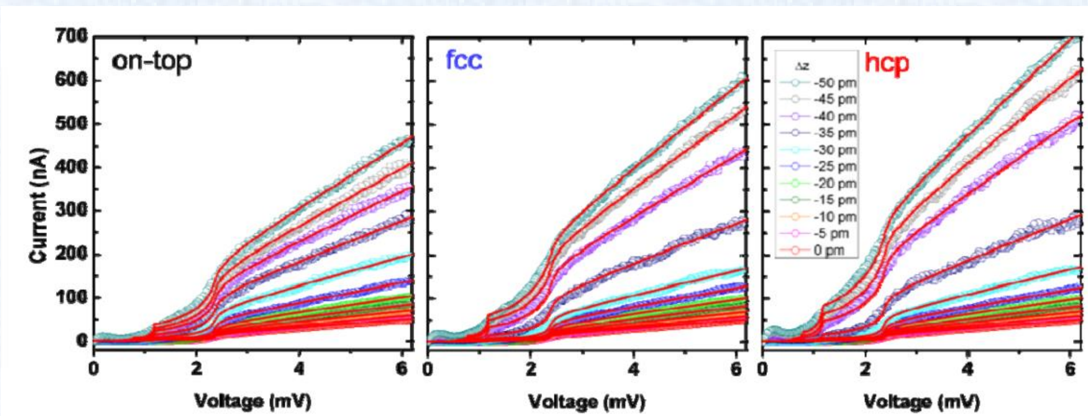


$\frac{2\Delta}{e}$ $\frac{2\Delta}{2e}$ $\frac{2\Delta}{3e}$



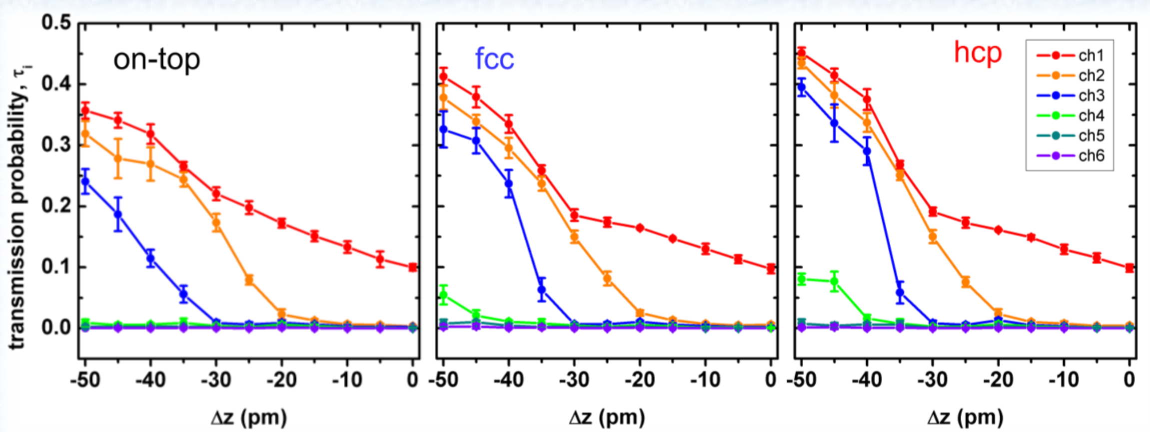
Observed channel and Objective

Fit : Multiple Andreev reflection formula → observed I–V



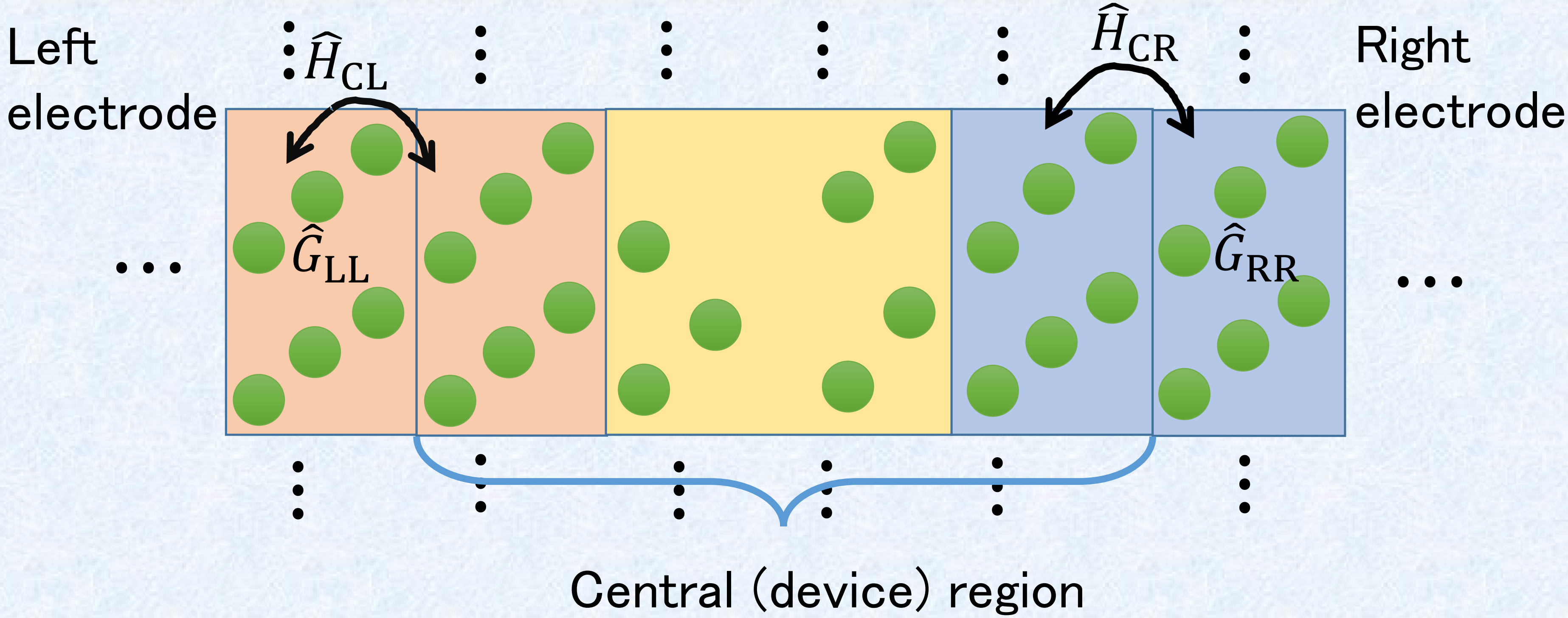
fcc vs hcp

Character of each channel
(atomic orbital, spatial distribution)



Microscopic picture
from a first-principles calculation

Transmission between semi-infinite electrode



$$\hat{G}_{\mathrm{C}}(E) = \{E - \hat{H}_{\mathrm{C}} - \hat{\Sigma}_{\mathrm{L}}(E) - \hat{\Sigma}_{\mathrm{R}}(E)\}^{-1}$$

$$\hat{\Sigma}_L(E) = \left(E - \hat{H}_{CL}\right)\hat{G}_{LL}\left(E - \hat{H}_{LC}\right)$$

$$\rho(r) = \frac{i}{2\pi}\int_{-\infty}^{\infty} dE\,[G_C(r,r,E+i0) - G_C(r,r,E-i0)]f(\mu - E)$$

$\hat{H}_{\mathrm{C}}$ $V_{KS}(r)$ $\rho_{\mathrm{periodic}}(r)$

Conductance and eigenchannel

Current

$$J = \int \frac{dE}{2\pi} \mathrm{Tr}\left[\hat{T}(E)\right]\{f(E-\mu_\mathrm{L}) - f(E-\mu_\mathrm{R})\}$$

$$\hat{T}(E) = \hat{G}_\mathrm{C}(E)\hat{\Gamma}_\mathrm{L}(E)\hat{G}_\mathrm{C}^\dagger(E)\hat{\Gamma}_\mathrm{R}(E)$$

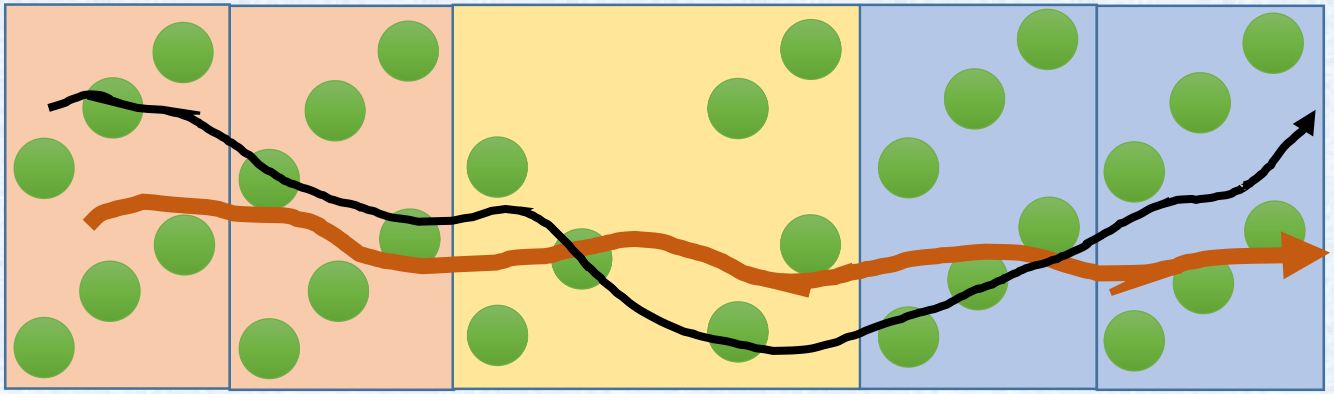
Nearlly zero bias→

$$J \propto \mathrm{Tr}\left[\hat{T}(0)\right](\mu_\mathrm{L} - \mu_\mathrm{R})$$

Conductance

Eigenchannel M. Paulsson and M. Brandbyge, PRB 76, 115117 (2007).

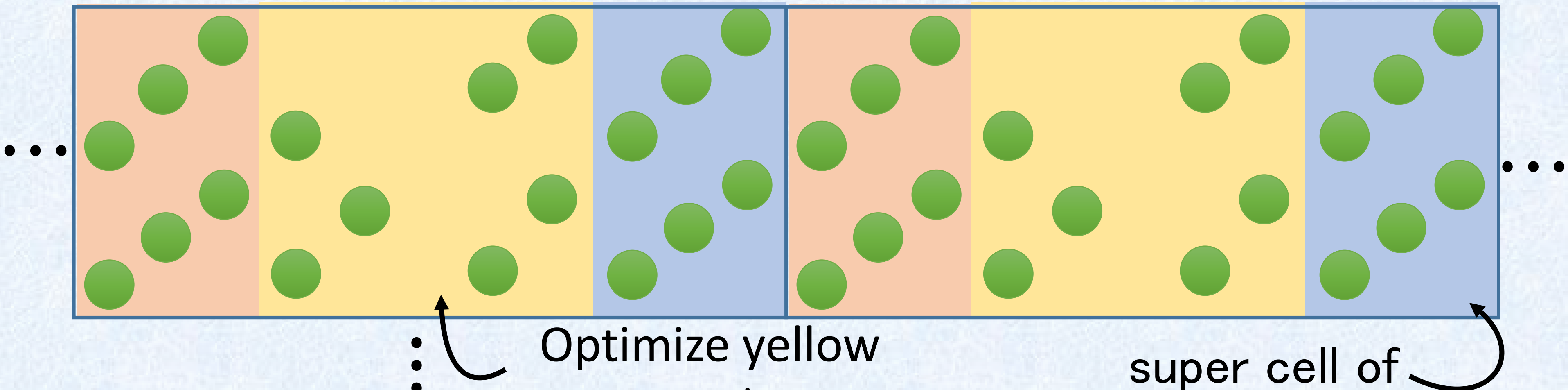
$$\hat{T}(E)|t_i(E)\rangle = t_i(E)|t_i(E)\rangle \qquad \mathrm{Tr}\left[\hat{T}(E)\right] = \sum_i t_i$$



Visualize transmission path

Numerical procedure and condition

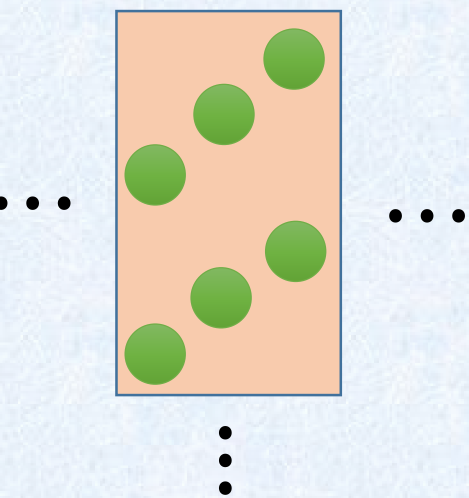
(1) Structure optimization of slab model (periodic)



Optimize yellow region only

super cell of 4×4 Pb(111) unit (48 atoms, Hex)

(2) Electrode(periodic)



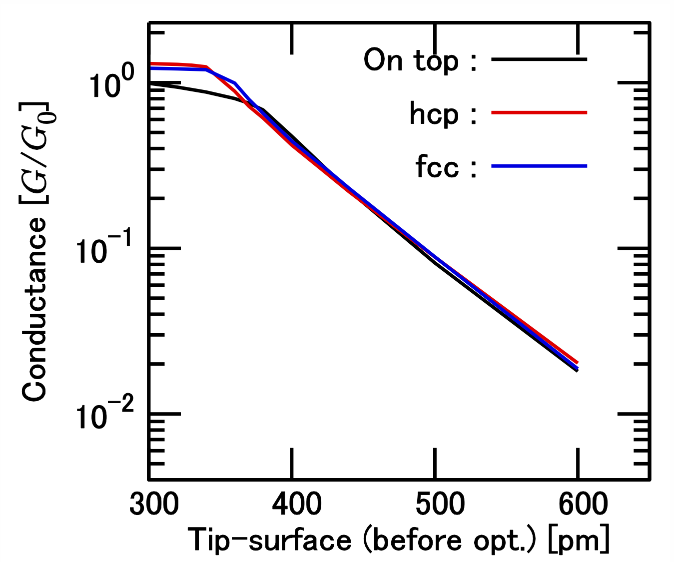
(3) Device green's function

Numerical conditions

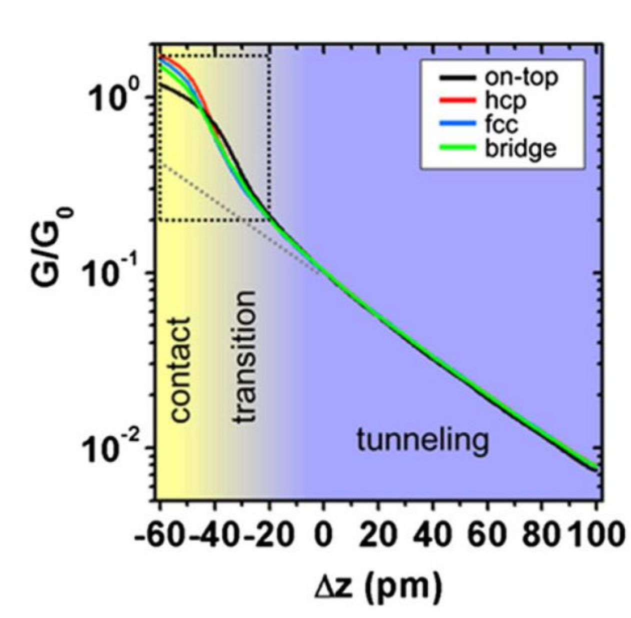
- OpenMX (Localized basis set + Pseudo potential) (Project for advancement of software usability@ISSP)
- GGA-PBE functional
- k points:2×2×1(1)、2×2×200(2)、2×2(3)
- Smearing: 1600 K (0.01 Ry)
- Basis: Pb8.0-s3p3d3f2 (Empty atoms on surface)
- Ignore Spin-Orbit interaction

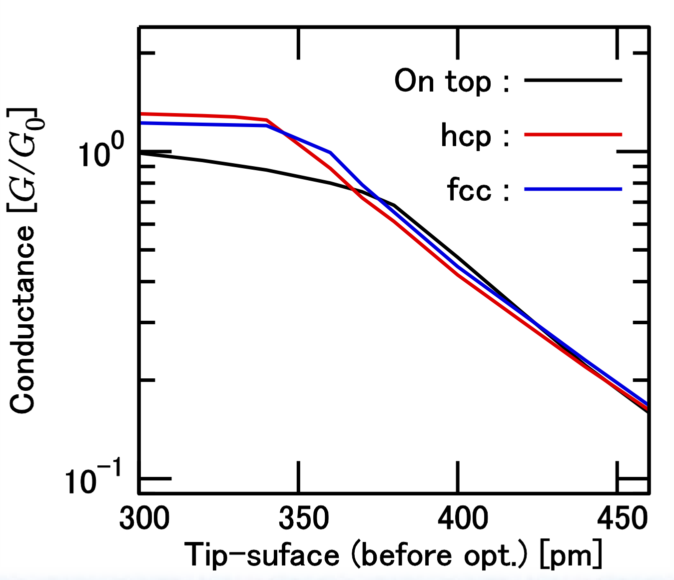
Conductance

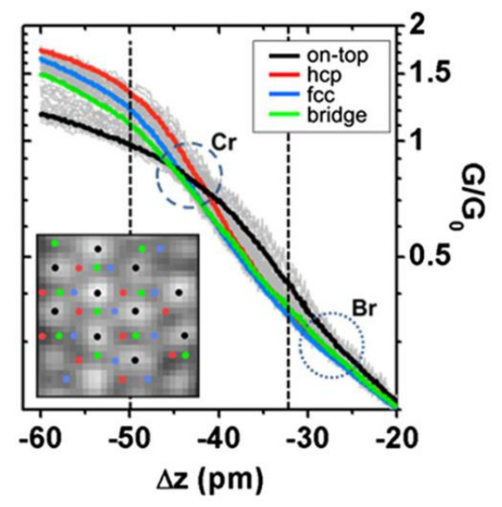
Result



H. Kim and Y. Hasegawa, PRL 114, 206801 (2015)

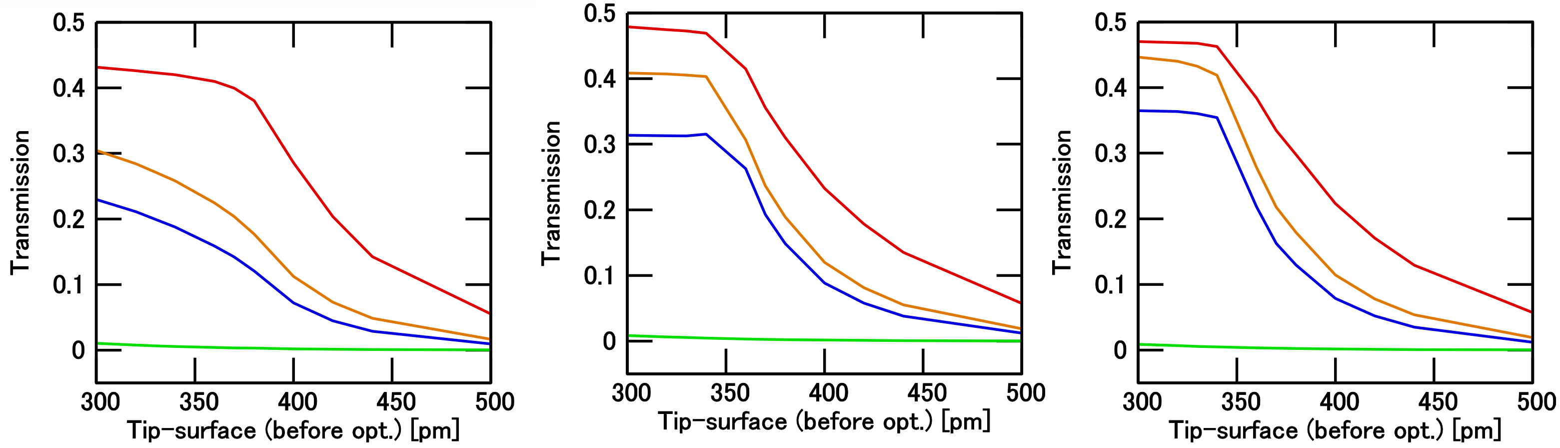




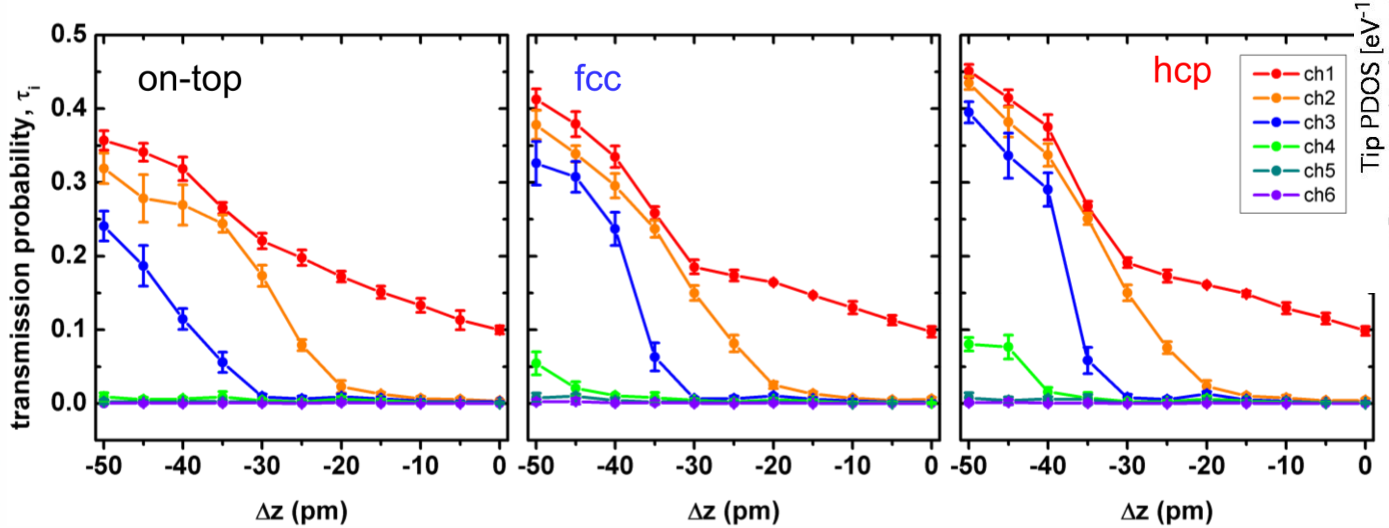


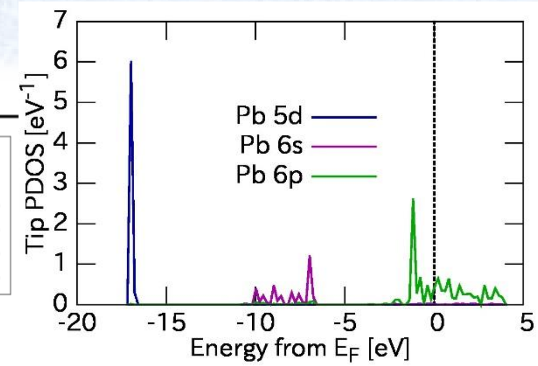
Transmission probability of each channel

Result



Experiment

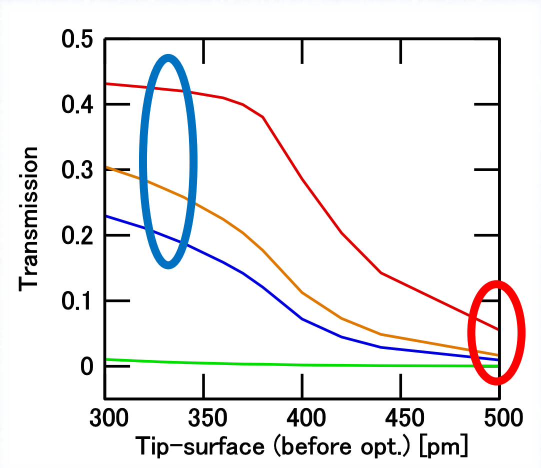


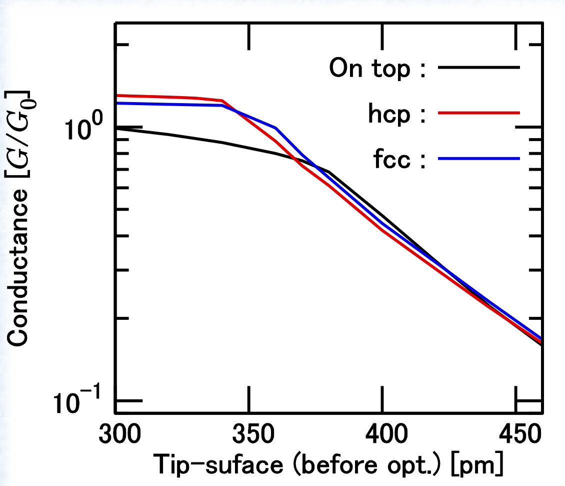


Result

Eigenchannels (on-top)

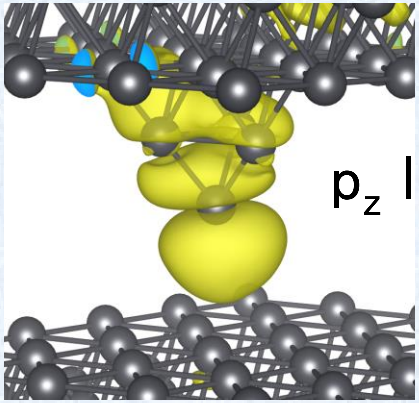
on-top





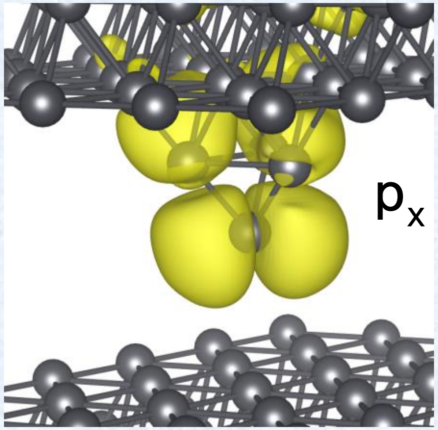
500 nm

1^{st} channel



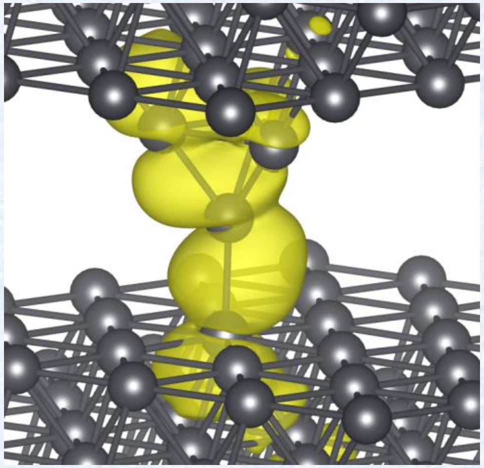
p_z like

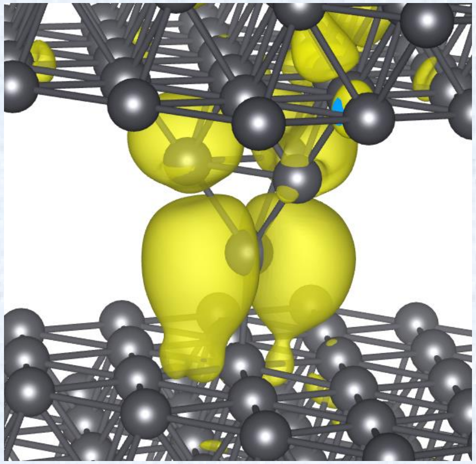
2^{nd} channel



p_x and p_y

330 nm



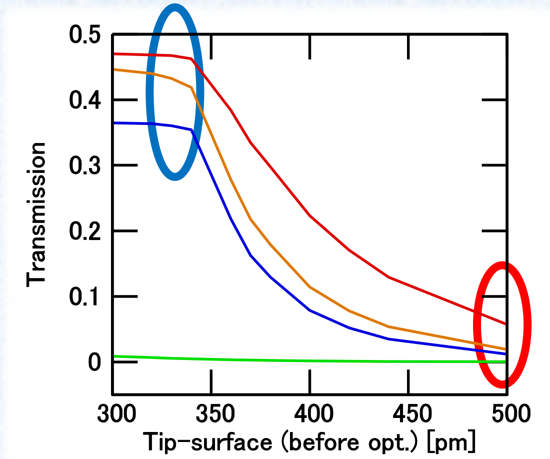


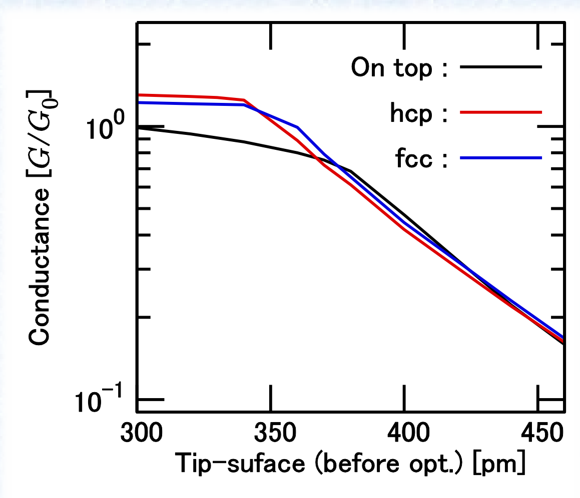
The same as 330 nm

Eigenchannels (hcp)

Result

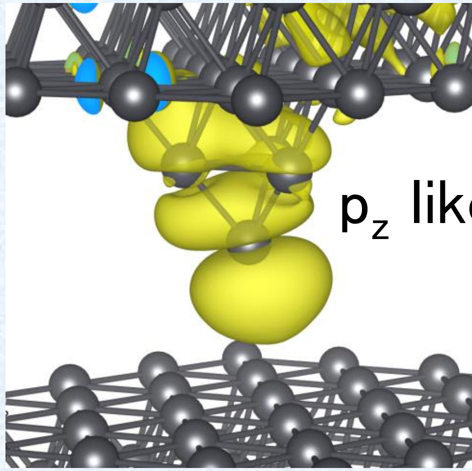
hcp





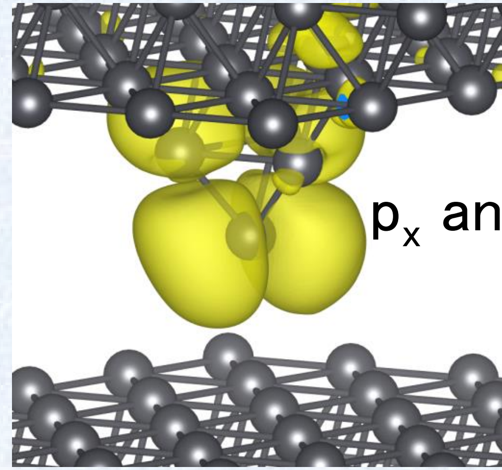
500 nm

1st channel



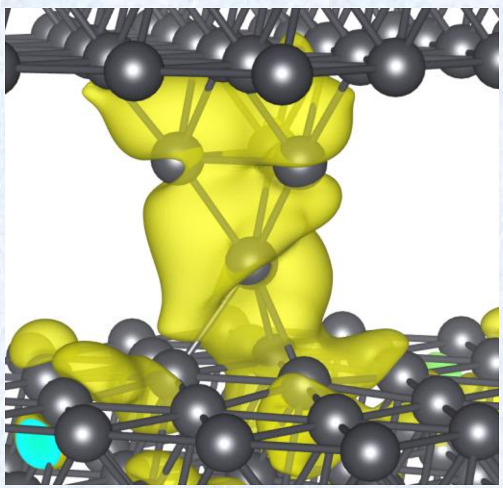
p_z like

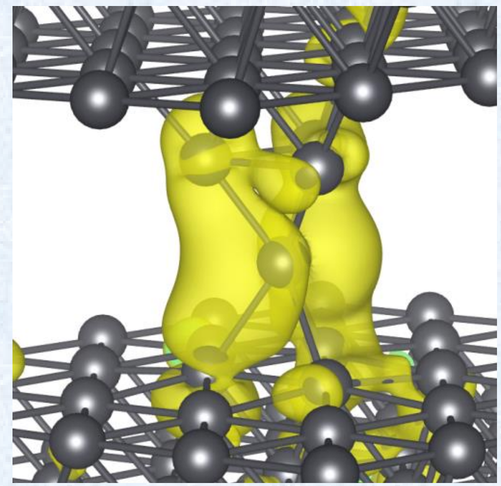
2nd channel



p_x and p_y

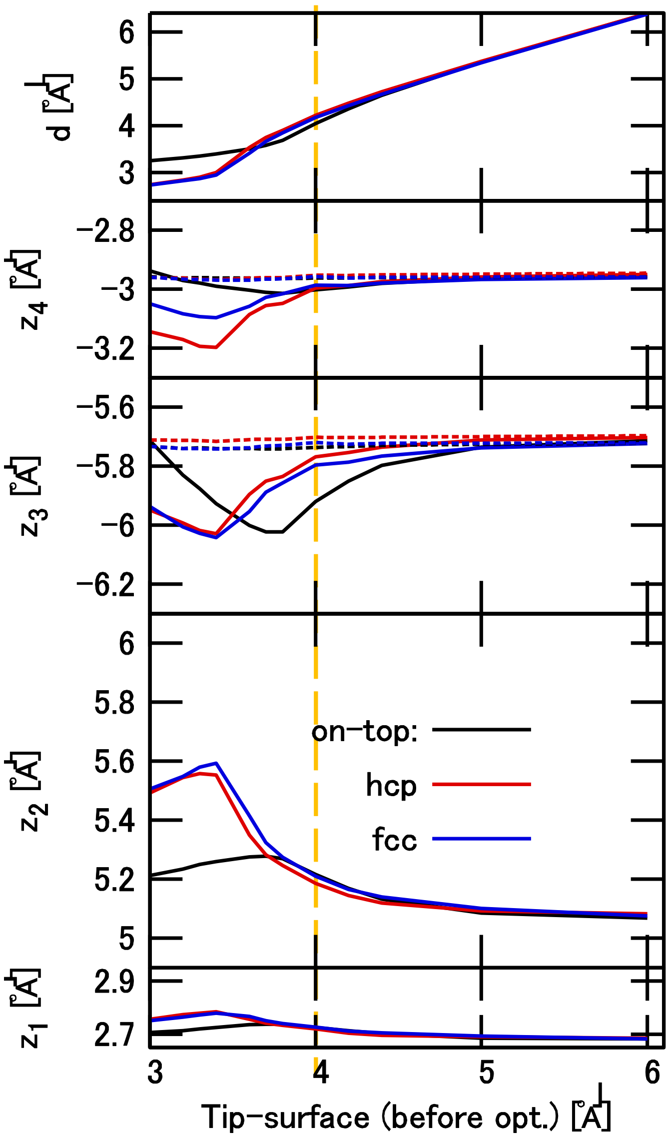
330 nm

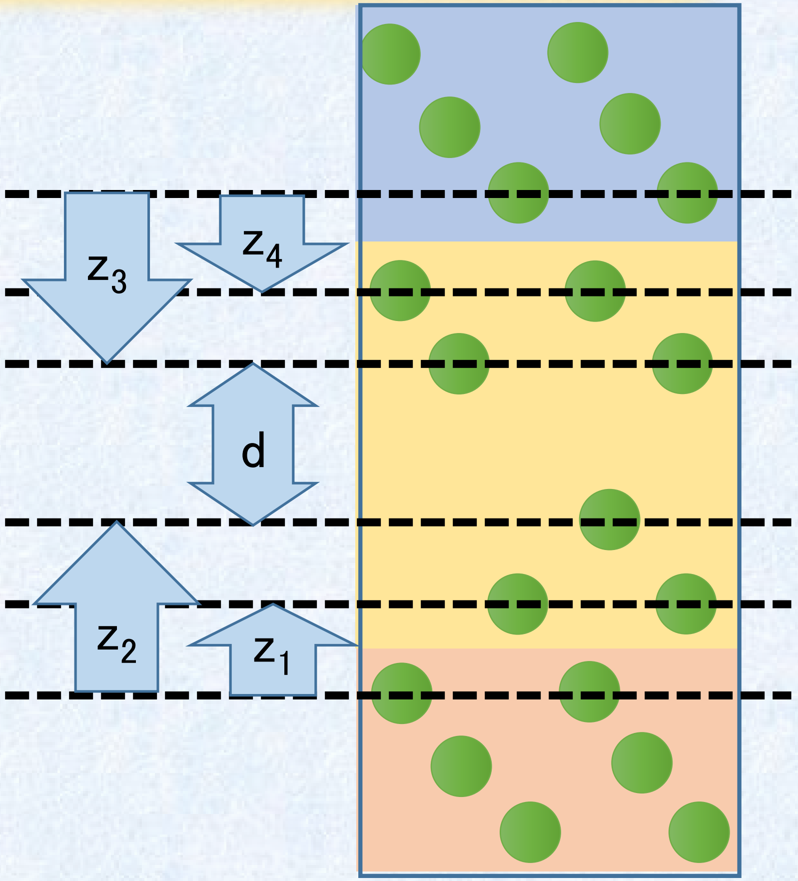




Hybridization with the surface orbital

Optimized structure (height of each layer)





About 4 Å: on−top has narrowest tip−surface

4 Å ～3 Å: Attraction of tip−surface

hcp/fcc ＞on−top

Summary 1

- We implemented a function for calculating eigenchannels in OpenMX (Project for advancement of software usage@ISSP).
- Conductance and eigenchannels in STM experiment of Pb(111)surface-Pb tip are reproduced semi-quantitatively.
- We explained the relation between spatial distribution of eigenchannels and tip-surface structure.

Outline

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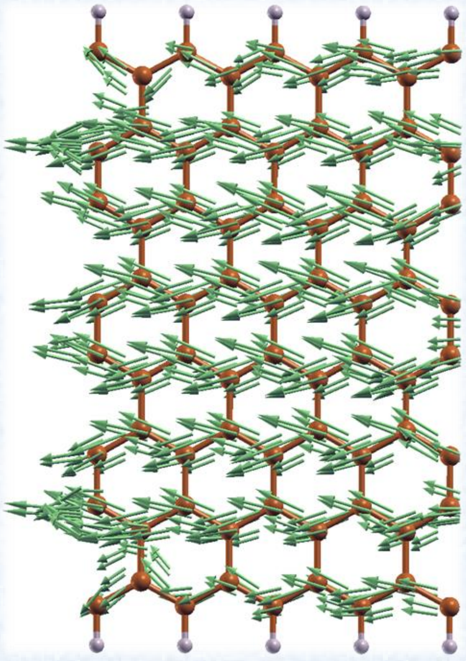


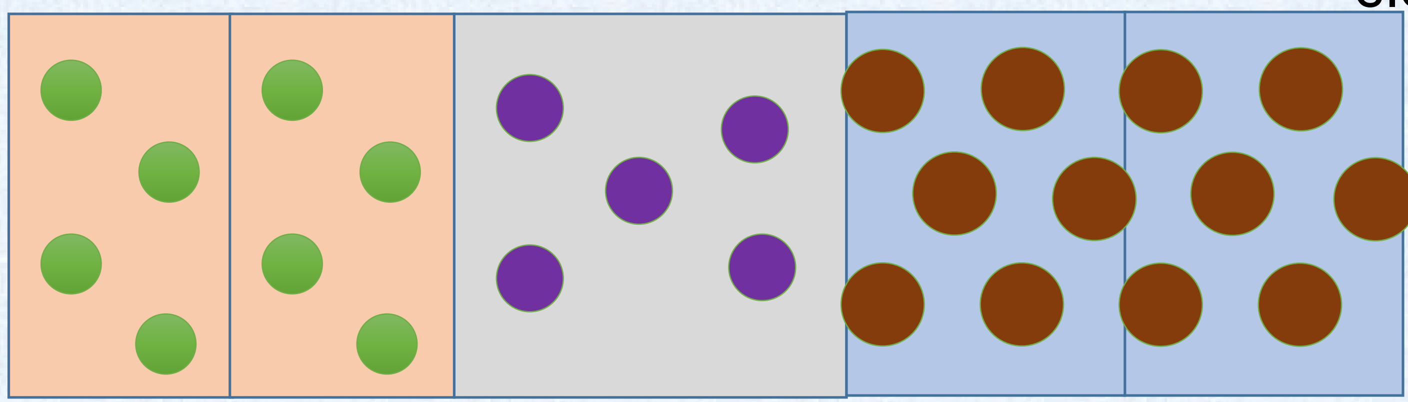
intro

Currentdensity in nanosystem

$$\boldsymbol{J}(r) = \frac{i}{2}\sum\left[\psi_i(r)\nabla\psi_i^*(r) - \psi_i^*(r)\nabla\psi_i(r)\right]$$

Left electrode

…



…

Right electrode

C. Li, L. Wan, Y. Wei, and J. Wang, Nanotechnology 19, 155401 (2008).

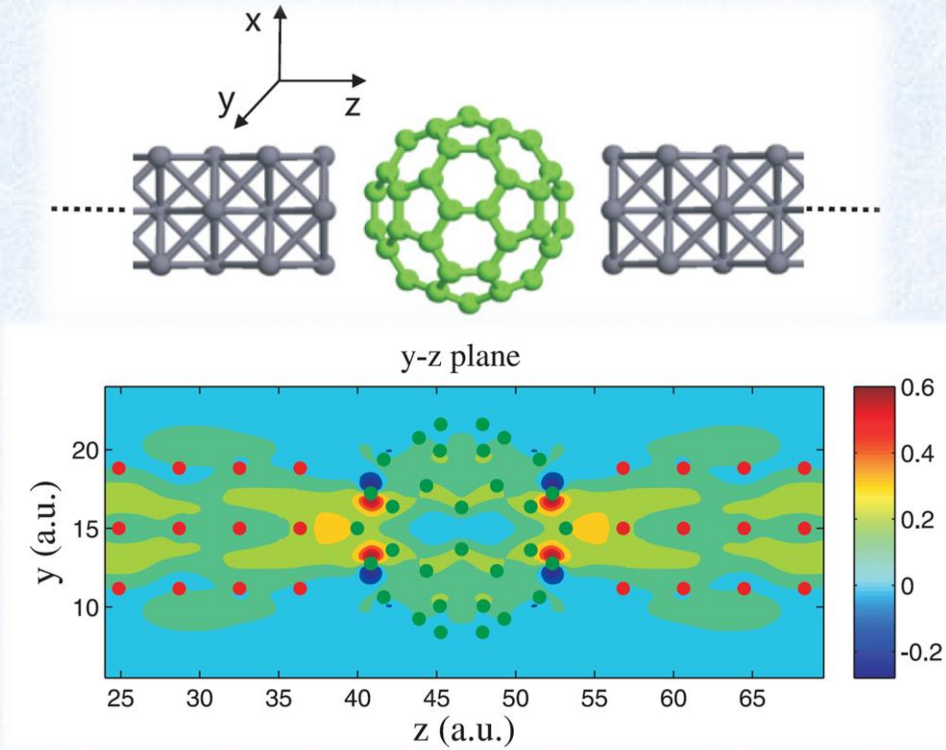
＋Correction for the Non-local potential

Hybrid functional

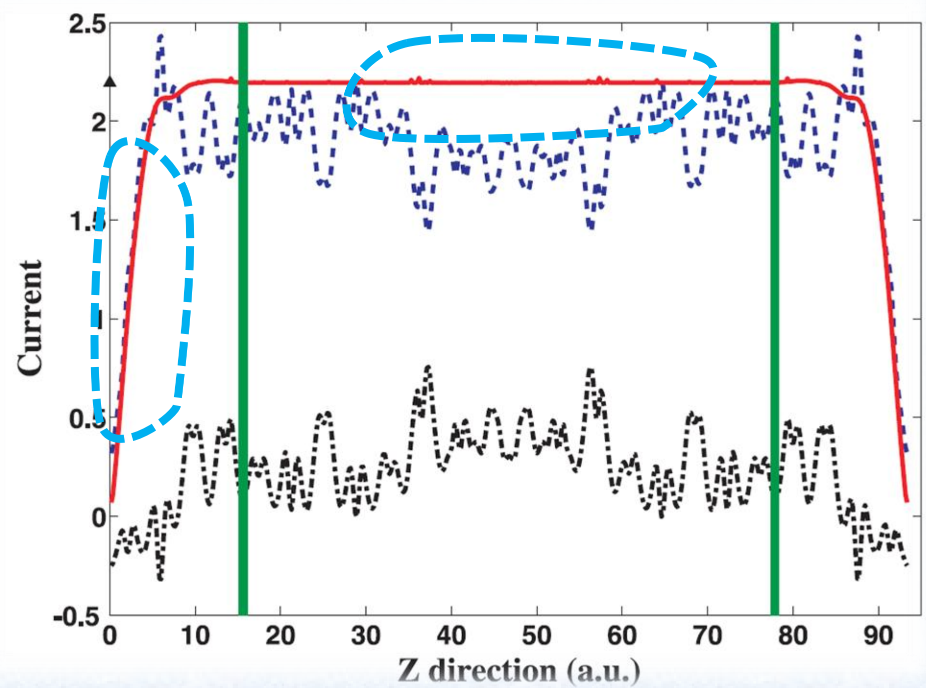
Pseudopotentails

$$\sum B_{ij}\,|\beta_i\rangle\langle\beta_j|$$

Conventional method



Lei Zhang, *et al*., PRB 84, 115412 (2011).



- Source and drain from electrodes
- Identical to the result of the Landauer formula at the center

In practice, it is hard for OpenMX

Objective: Avoiding this difficulty.

method

Currentdensity witn non-local potential

With non-local potential

$$i\frac{\partial\psi(r,t)}{\partial t}=\frac{-\nabla^2}{2}\psi(r,t)+\int d^3r'\,V(r,r')\psi(r',t)\quad(1)$$

Hybrid functional

Pseudopotentails

$$\sum B_{ij}\,|\beta_i\rangle\langle\beta_j|$$

$$\psi^*(r,t)\times(1)-\psi(r,t)\times(1)^*$$

$$-\frac{\partial\rho(r,t)}{\partial t}=\nabla\cdot\boldsymbol{J}_{\mathrm{Loc}}(r,t)+\rho_{\mathrm{NLoc}}(r,t)$$

$$\boldsymbol{J}_{\mathrm{Loc}}(r,t)\equiv\frac{i}{2}[\psi(r,t)\nabla\psi^*(r,t)-\psi^*(r,t)\nabla\psi(r,t)]$$

$$\rho_{\mathrm{NLoc}}(r,t)\equiv i\int d^3r'\,V(r,r')\psi(r',t)\psi^*(r,t)-\mathrm{c.c.}$$

C. Li, L. Wan, *et al.*, Nanotechnology **19**, 155401 (2008).

$$\boldsymbol{J}_{\mathrm{NLoc}}(r,t)\equiv\nabla\cdot\varphi_{NLoc}(r,t)$$

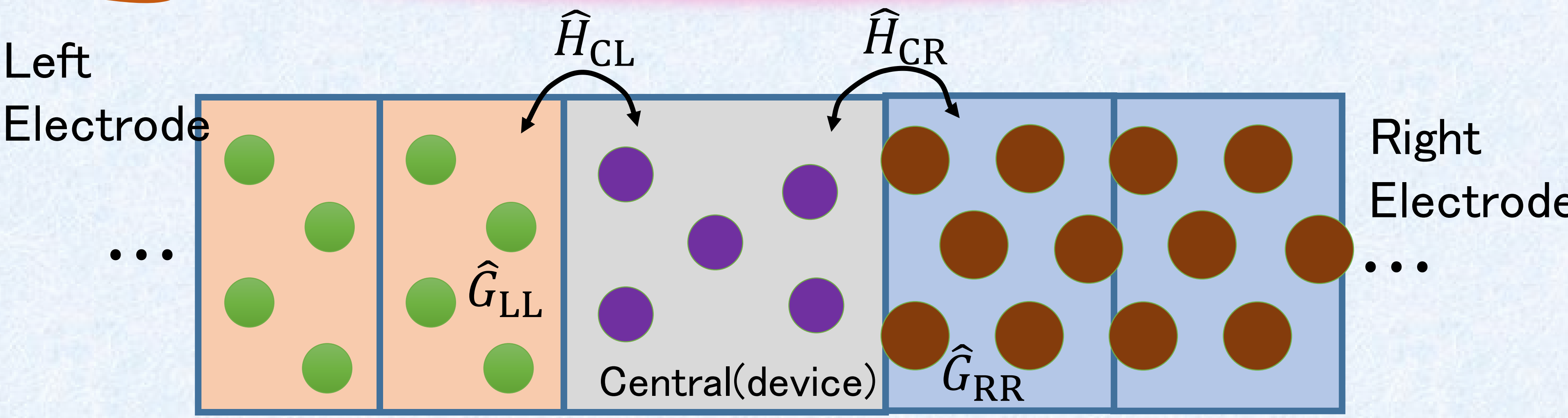
$$-\frac{\partial\rho(r,t)}{\partial t}=\nabla\cdot[\boldsymbol{J}_{\mathrm{Loc}}(r,t)+\boldsymbol{J}_{\mathrm{NLoc}}(r,t)]$$

$$\nabla^2\varphi_{\mathrm{NLoc}}(r,t)=\rho_{\mathrm{NLoc}}(r,t)$$

Poisson eq.

method

Currentdensity in NEGF



L. V. Keldysh, Sov. Phys. JETP 20, 1018 (1965). T. Ozaki, et al., PRB 81, 035116 (2010).

$$\hat{G}_{\mathrm{C}}(E) = \{E - \hat{H}_{\mathrm{C}} - \hat{\Sigma}_{\mathrm{L}}(E) - \hat{\Sigma}_{\mathrm{R}}(E)\}^{-1}$$

$$\hat{\Sigma}_L(E) = (E - \hat{H}_{CL})\hat{G}_{LL}(E - \hat{H}_{LC})$$

$$\hat{\Gamma}_L \equiv \mathrm{Im}[\Sigma_L]$$

Total current:

$$J = \int \frac{dE}{2\pi} \mathrm{Tr}\left[\hat{G}_{\mathrm{C}}(E)\hat{\Gamma}_L(E)\hat{G}_{\mathrm{C}}(E)\hat{\Gamma}_R(E)\right]\{f(E-\mu_{\mathrm{L}}) - f(E-\mu_{\mathrm{R}})\}$$

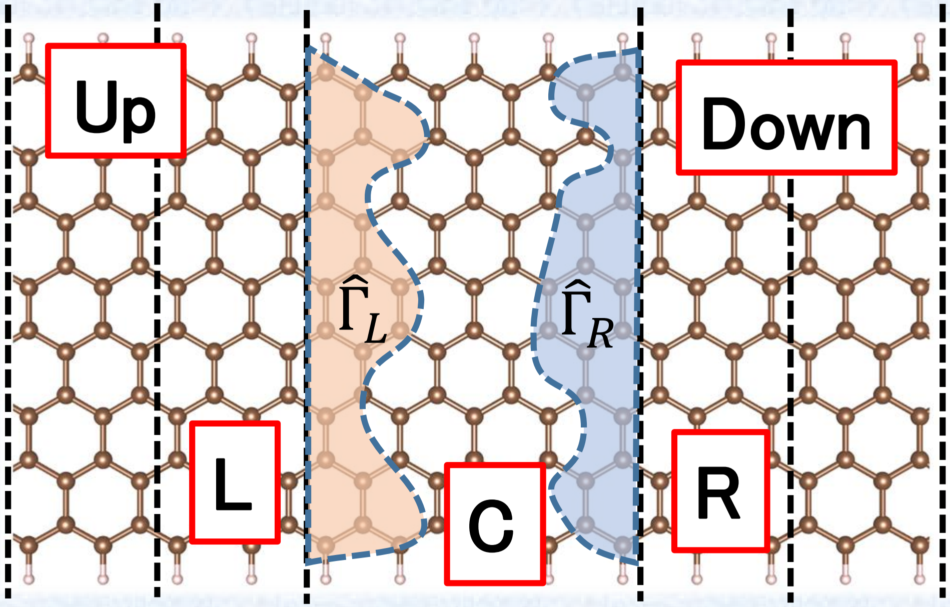
Currentdensity:

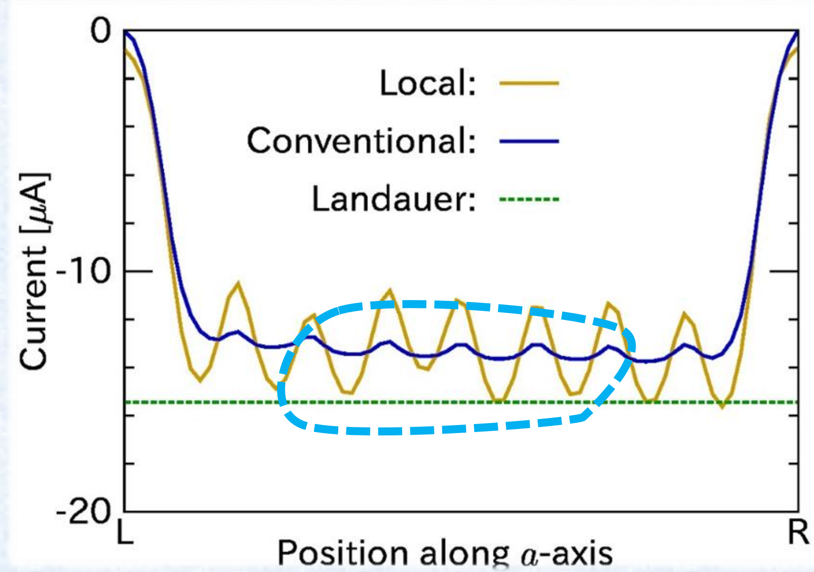
$$\boldsymbol{J}_{\mathrm{Loc}}(r) = \sum_{ij}\left[\hat{G}_C\hat{\Gamma}_R\hat{G}_C\right]_{ij}\left[\chi_j(r)\nabla\chi_i(r) - \chi_i(r)\nabla\chi_j(r)\right]\left[f(E-\mu_L) - f(E-\mu_R)\right]$$

$$\rho_{\mathrm{NLoc}}(r) = -2\sum_{ij}\left[\hat{V}\hat{G}_{C}\hat{\Gamma}_{R}\hat{G}_{C}\right]_{ij}\chi_i(r)\chi_j(r)\left[f(E-\mu_L) - f(E-\mu_R)\right]$$

Lei Zhang, *et al.*, PRB 84, 115412 (2011).

Result of the conventional method

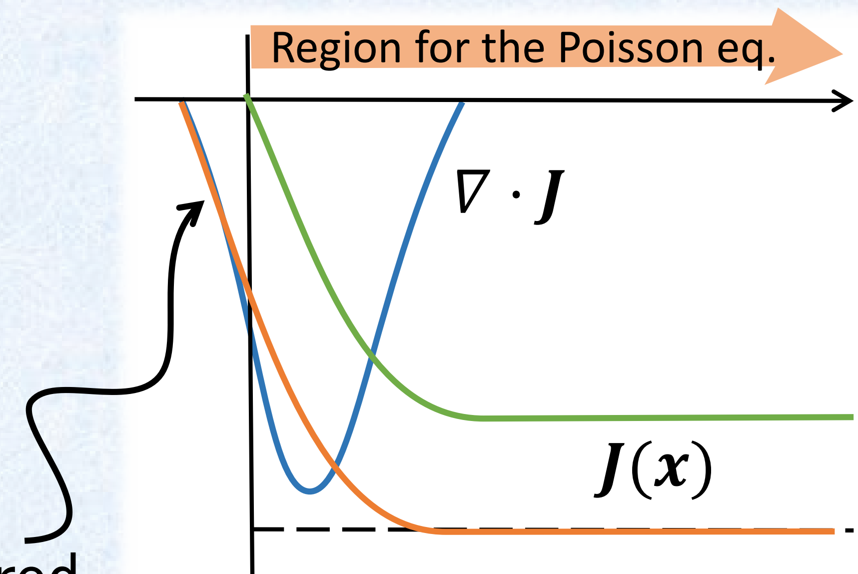




Inconsistent with the Landauer formula

Source and drain
by the coupling to electrodes
$\nabla \cdot \boldsymbol{J}$ is given

$$J(x) = J(0) + \int_0^x dx' \frac{dJ(x')}{dx'}$$



Contribution from this region is ignored

Solution

Obtain $\nabla \cdot \boldsymbol{J}$ through a different route

the continuity equation $-\frac{\partial \rho(r,t)}{\partial t} = \nabla \cdot \boldsymbol{J}_{\mathrm{Loc}}(r,t) + \rho_{\mathrm{NLoc}}(r,t)$

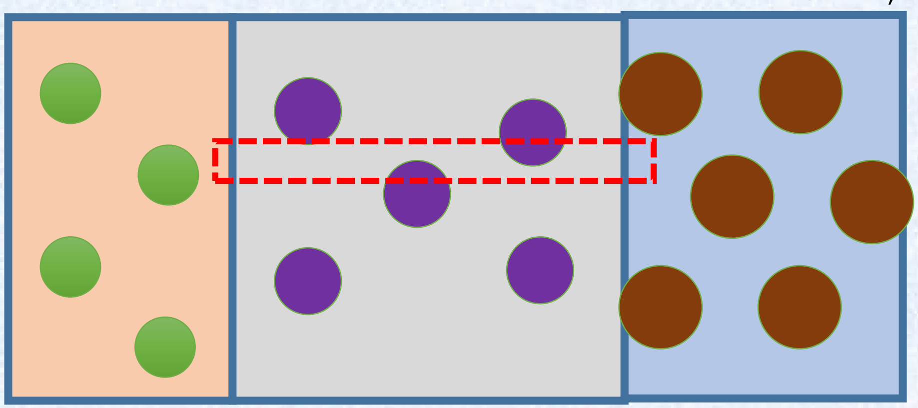
In the steady state

$$\rho_{\mathrm{NLoc}}(r) = -\nabla \cdot \boldsymbol{J}_{\mathrm{Loc}}(r)$$

Boundary condition for the Poisson eq.

$$J = \int \frac{dE}{2\pi}\{f(E-\mu_{\mathrm{L}}) - f(E-\mu_{\mathrm{R}})\}\sum_{ij}\left[\hat{G}_{\mathrm{C}}(E)\hat{\Gamma}_{L}(E)\hat{G}_{\mathrm{C}}(E)\hat{\Gamma}_{R}(E)\right]_{ij}\int d^2x_{\perp}\,\chi_i(r)\chi_j(r)$$

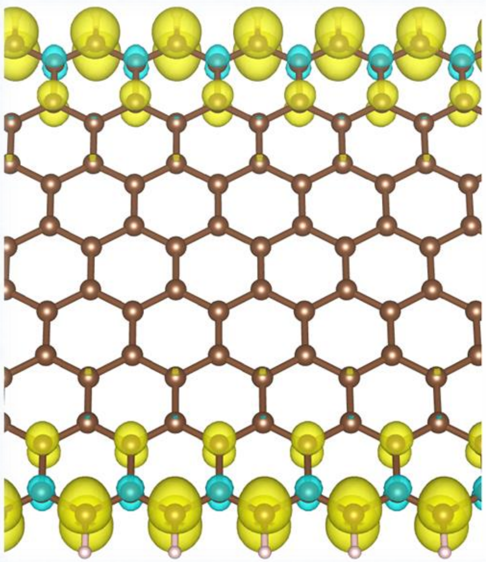
C. Li, L. Wan, *et al.*, Nanotechnology **19**, 155401 (2008).



Force identical to the Landauer formula at boundaries

Identical in whole region

8–Zigzag graphene nanoribbon



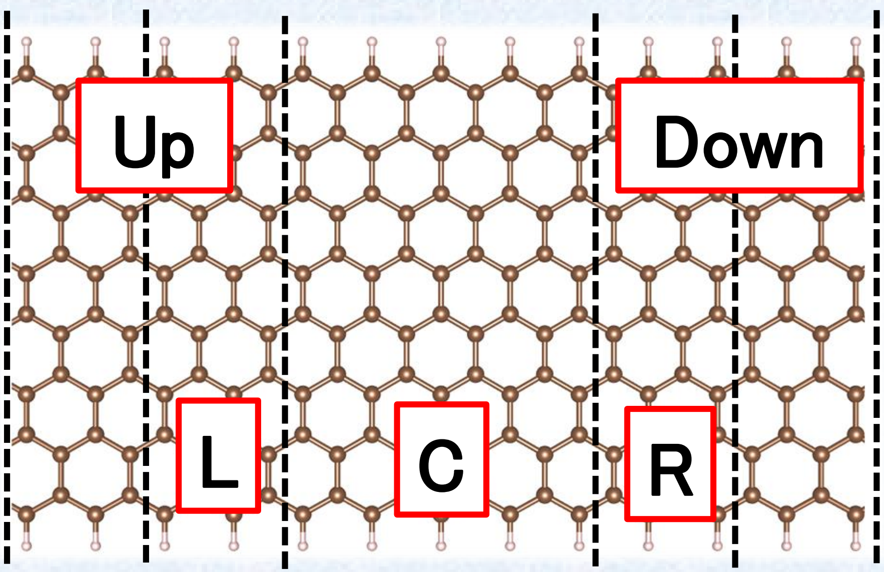
Numerical conditions

- OpenMX (Software Advancement Project@ISSP)
- LDA-PZ functional
- Norm-conserving PP
- Basis: C5.0-s2p1, H5.0-s2
- PW cutoff (Poisson eq.): 120 Ry
- Smearing: 300 K

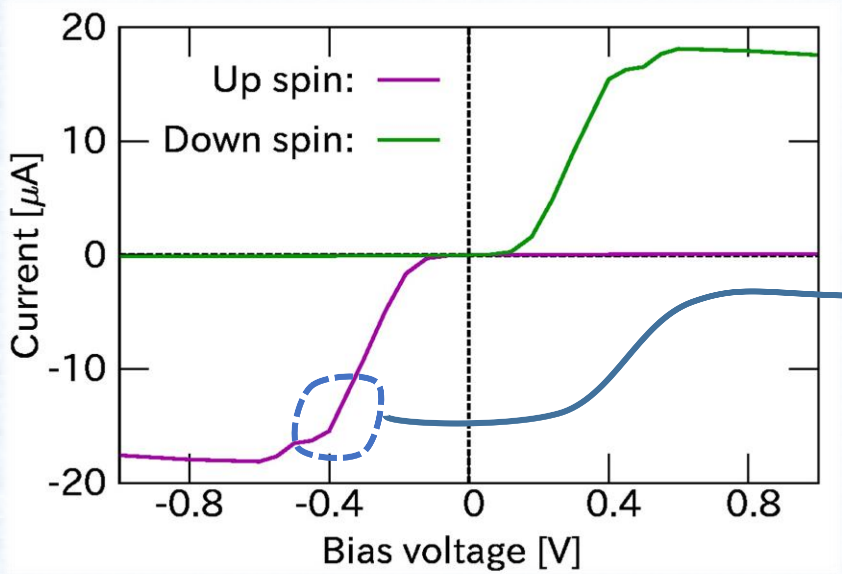
Magnetization: $0.24\mu_{\mathrm{B}}$ /edge/cell

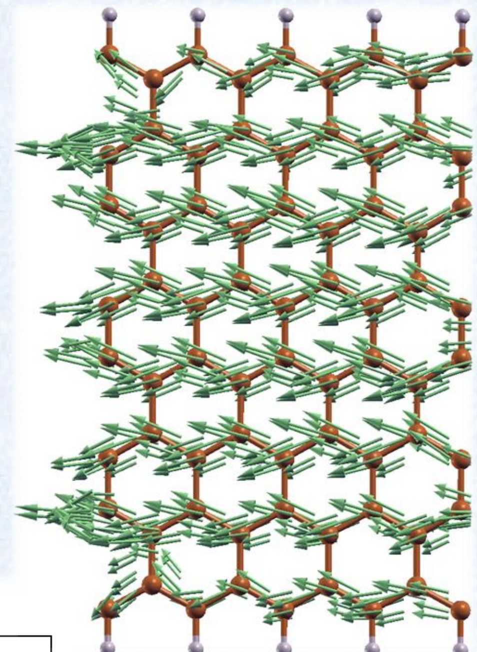
- Magnetic moment at edges
- Spin filter effect (Domain wall)

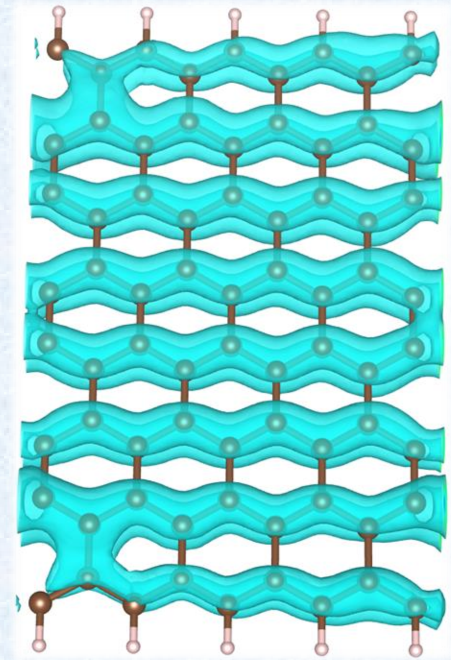
T. Ozaki, *et al.*, PRB 81, 075422 (2010).

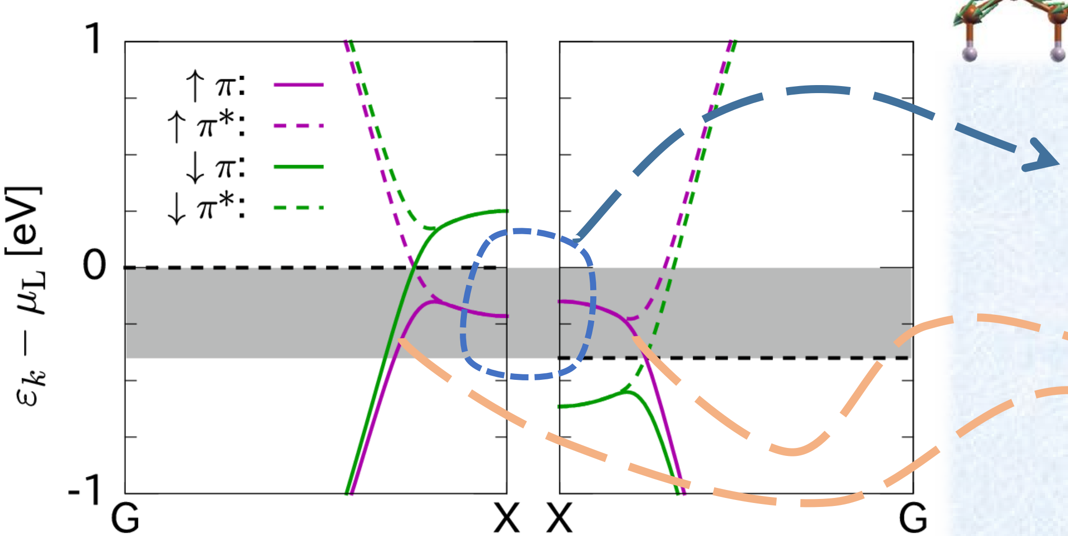


Currentdensity







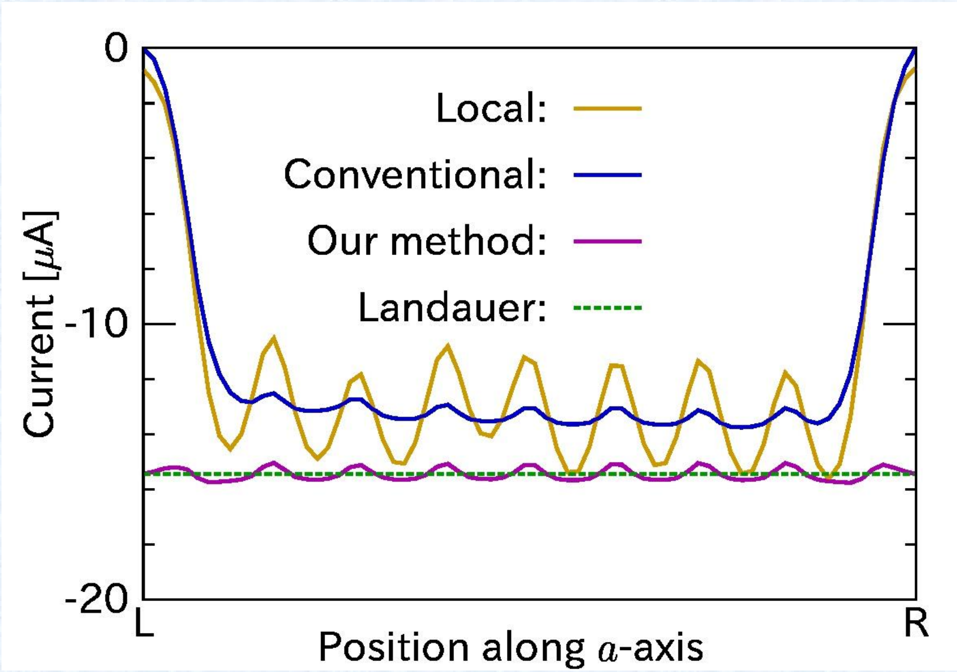


Localized at edge

Delocalized

result

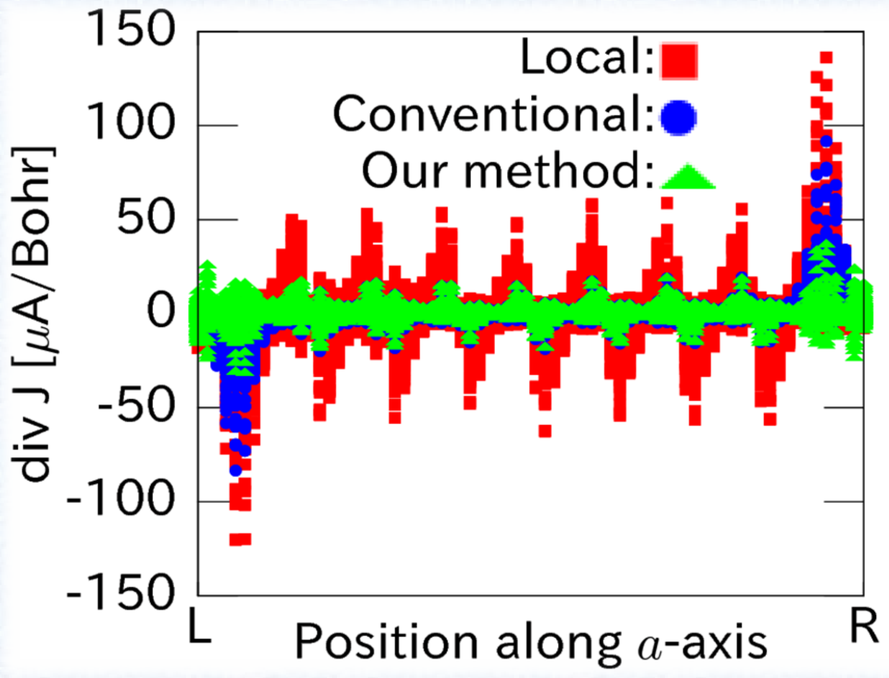
Conservation of currentdensity



Local: Effect of non-local potential in the vicinity of C atoms.

Our method: Identical to the Landauer formula at each slice.

Conserved currentdensity



Summary

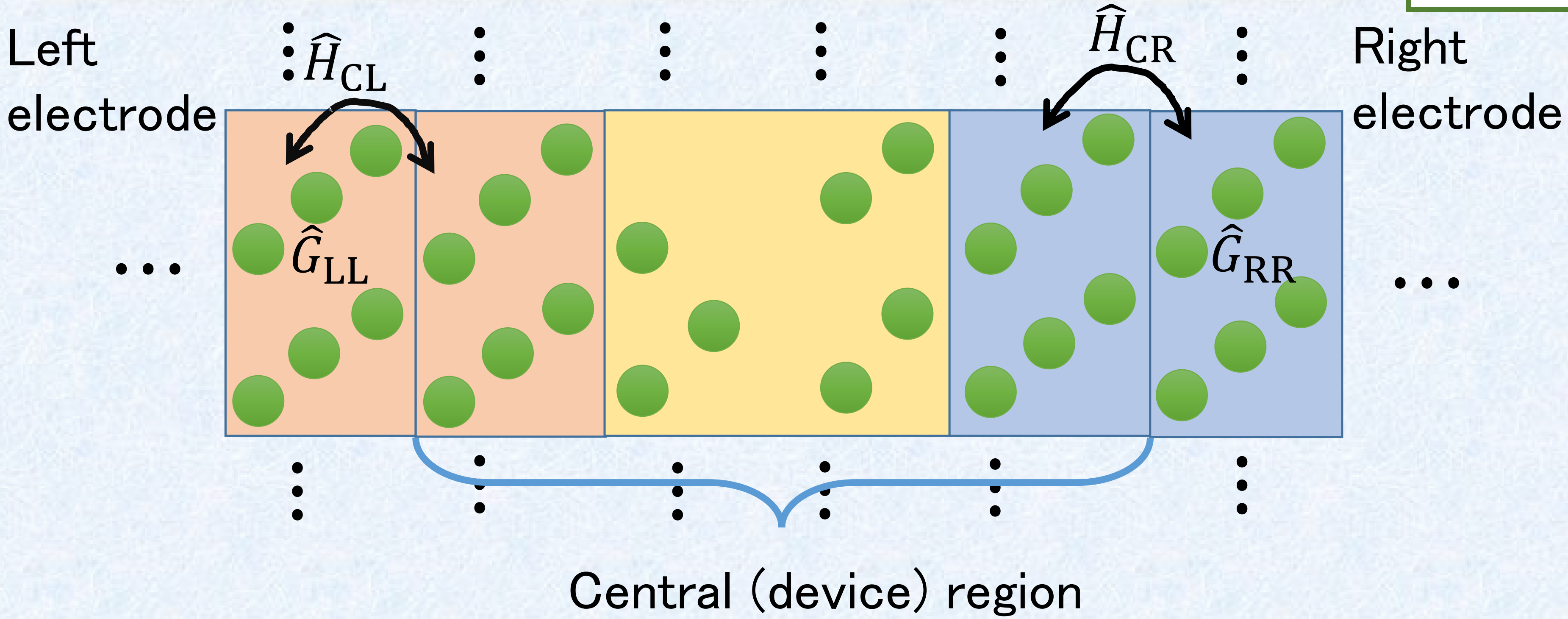
- When we implement the conventional method for the currentdensity into OpenMX, there is a difficulty in the Poisson equation for computing non-local current.
- We developed a new method for computing non-local term with the aid of the continuity equation. And we implement this method into OpenMX (Software advancement project).
- We applied this method to 8-Zigzag graphene nanoribbon.
- Targets
  - (Anisotropic) tunnel magneto-resistance device.
  - Graphene (nanoribbon)
  - SiC
  - Etc…

・・・ We can also compute the non-collinear spin currentdensity

$J_{\sigma\sigma'}(r)$ 3×3 matrix at each spatial point(spin×velocity)

Transmission between semi-infinite electrode

theory



$$\begin{pmatrix} \hat{H}_L & \hat{H}_{LC} & 0 \\ \hat{H}_{CL} & \hat{H}_C & \hat{H}_{CR} \\ 0 & \hat{H}_{RC} & \hat{H}_R \end{pmatrix} \begin{pmatrix} |\psi_L\rangle \\ |\psi_C\rangle \\ |\psi_R\rangle \end{pmatrix} = E \begin{pmatrix} |\psi_L\rangle \\ |\psi_C\rangle \\ |\psi_R\rangle \end{pmatrix} \qquad \hat{H}_L|\varphi_n\rangle = E|\varphi_n\rangle$$

$$\begin{pmatrix} |\psi_L\rangle \\ |\psi_C\rangle \\ |\psi_R\rangle \end{pmatrix} = \begin{pmatrix} |\varphi_n\rangle + \hat{G}_{LC}\hat{H}_{CL}|\varphi_n\rangle \\ \hat{G}_C\hat{H}_{CL}|\varphi_n\rangle \\ \hat{G}_{RC}\hat{H}_{CL}|\varphi_n\rangle \end{pmatrix} \quad \begin{pmatrix} \hat{G}_L & \hat{G}_{LC} & \hat{G}_{LR} \\ \hat{G}_{CL} & \hat{G}_C & \hat{G}_{CR} \\ \hat{G}_{RL} & \hat{G}_{RC} & \hat{G}_R \end{pmatrix} \equiv \left[E - \begin{pmatrix} \hat{H}_L & \hat{H}_{LC} & 0 \\ \hat{H}_{CL} & \hat{H}_C & \hat{H}_{CR} \\ 0 & \hat{H}_{RC} & \hat{H}_R \end{pmatrix} \right]^{-1}$$

Detail for calsurating eigenchannel

$|t_i(E)\rangle$:Special superposition of

M. Paulsson and M. Brandbyge, PRB 76, 115117 (2007).

$\hat{G}_{\mathrm{C}}\hat{\Gamma}_{\mathrm{L}}\hat{G}_{\mathrm{C}}^{\dagger}$ Spectral function

$$\hat{A}_{\mathrm{L}}\hat{\Gamma}_{\mathrm{R}}|t_i\rangle = t_i|t_i\rangle$$

Hermite

$$\hat{A}_{\mathrm{L}}|a_i\rangle = a_i|a_i\rangle$$

$$\hat{A}_{\mathrm{L}}^{1/2} \equiv (\sqrt{a_1}\,|a_1\rangle, \cdots, \sqrt{a_N}\,|a_N\rangle)$$

$$\hat{A}_{\mathrm{L}}^{1/2}\hat{A}_{\mathrm{L}}^{1/2\dagger}\hat{\Gamma}_{\mathrm{R}}\hat{A}_{\mathrm{L}}^{1/2}\hat{A}_{\mathrm{L}}^{-1/2}|t_i\rangle = t_i\hat{A}_{\mathrm{L}}^{1/2}\hat{A}_{\mathrm{L}}^{-1/2}|t_i\rangle$$

$$\hat{\tilde{\Gamma}}_{\mathrm{R}}|\tilde{t}_i\rangle = t_i|\tilde{t}_i\rangle$$

$$|t_i\rangle = \hat{A}_{\mathrm{L}}^{1/2}|\tilde{t}_i\rangle$$

In the real space

$$t_i(r) = [\chi_1(r), \cdots, \chi_N(r)]|t_i\rangle$$

In OpenMX $\int d^3r\,\chi_i(r)\chi_j(r) \neq \delta_{ij}$

Löwdin orthogonalizations

The Kohn-Shame eqn. in the non-orthogonal basis space

$$\hat{H}|\varphi_i\rangle = \varepsilon_i \hat{S}|\varphi_i\rangle \qquad S_{ij} \equiv \int d^3r\, \chi_i(r)\chi_j(r)$$

Solve directly Generalized Eigenvalue Problem

Löwdin ort.

$$\hat{H}\hat{S}^{-1/2\dagger}\hat{S}^{1/2\dagger}|\varphi_i\rangle = \varepsilon_i \hat{S}^{1/2}\hat{S}^{1/2\dagger}|\varphi_i\rangle$$

$$\hat{S}|s_i\rangle = s_i|s_i\rangle$$

$$\hat{S}^{1/2} \equiv \left(\sqrt{s_1}\,|s_1\rangle, \cdots, \sqrt{s_N}\,|s_N\rangle\right)$$

$$\hat{S}^{-1/2\dagger} \equiv \left(s_1^{-1/2}\,|s_1\rangle, \cdots, s_N^{-1/2}|s_N\rangle\right)$$

$$\tilde{\hat{H}}|\tilde{\varphi}_i\rangle = \varepsilon_i|\tilde{\varphi}_i\rangle$$

$$\tilde{\hat{H}} = \hat{S}^{-1/2}\hat{H}\hat{S}^{-1/2\dagger}$$

$$|\varphi_i\rangle = \hat{S}^{-1/2\dagger}|\tilde{\varphi}_i\rangle$$

Others?

Löwdin ort. for $\hat{G}_\mathrm{C}$, $\hat{\Gamma}$, $\hat{T}$, eigenchannels

Hamiltonian $\hat{\tilde{H}} = \hat{S}^{-1/2}\hat{H}\hat{S}^{-1/2\dagger}$

Green's function $\hat{\tilde{G}} = \hat{S}^{1/2\dagger}\hat{G}\hat{S}^{1/2}$

Self energy
Line width $\hat{\tilde{\Gamma}} = \hat{S}^{-1/2}\hat{\Gamma}\hat{S}^{-1/2\dagger}$

Any vectors

$$|\varphi_i\rangle = \hat{S}^{-1/2\dagger}|\tilde{\varphi}_i\rangle$$

Basis set

$$\tilde{\chi}_n(r) = \sum_n \chi_n(r)\left[\hat{S}^{-1/2\dagger}\right]_{n'n}$$

$$\hat{\tilde{T}} = \hat{\tilde{G}}_\mathrm{C}\hat{\tilde{\Gamma}}_\mathrm{L}\hat{\tilde{G}}_\mathrm{C}^\dagger\hat{\tilde{\Gamma}}_\mathrm{R} = \hat{S}^{1/2\dagger}\hat{G}_\mathrm{C}\hat{\Gamma}_\mathrm{L}\hat{G}_\mathrm{C}^\dagger\hat{\Gamma}_\mathrm{R}\hat{S}^{-1/2\dagger}$$

Obtain it in the orthogonal basis space

$$\hat{\tilde{T}}(E)|\tilde{t}_i(E)\rangle = t_i(E)|\tilde{t}_i(E)\rangle$$

Diagonalize in the orthogonal basis space

$$|t_i\rangle = \hat{S}^{-1/2\dagger}|\tilde{t}_i\rangle$$

Transform to the non-orthogonal basis space