# Toward an O(N) method for the non-equilibrium Green's function calculation

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# Introduction

- Research purpose
  - Development of a program code of electron and spin transport calculation by Non Equilibrium Green's Function (NEGF) method for large scale systems
- Approach
  - Linear scaling NEGF method based on a divide-conquer (DC) approach
- Problem
  - Applying the DC approach[1] to the NEGF method[2] simply can make it hard to obtain accurate local Green's functions due to the influence of the dangling bonds of a truncated cluster.

[1] W. Yang, Phys. Rev. Lett. **66**, 1438 (1991); W. Yang and T. S. Lee, J. Chem. Phys. **103**, 5674 (1995).
[2] T. Ozaki, K. Nishio and H. Kino, Phys. Rev. B **81**, 035116 (2010).

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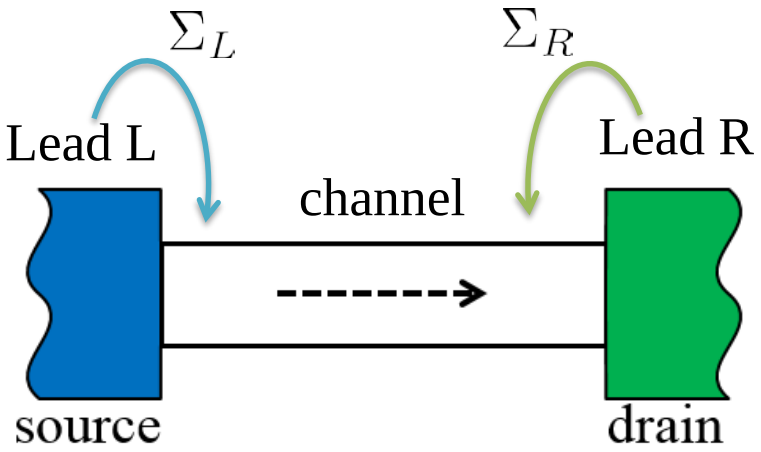
- Divide-conquer (DC) approach
- Examples
- Conclusion

# NEGF for electronic transportation




$$G(E) = [ES - H(\rho) - \Sigma_L(E) - \Sigma_R(E)]^{-1}$$

$$T(E) = \mathrm{Tr}\left[\Gamma_L(E)G(E)\Gamma_R(E)G^{\dagger}(E)\right]$$

Step 1 (Lead part)

(i) Electronic structure of the leads

(ii) Surface Green's function of the leads

(iii) Self energy

Step 2 (SCF part)

(i) Hamiltonian of the channel

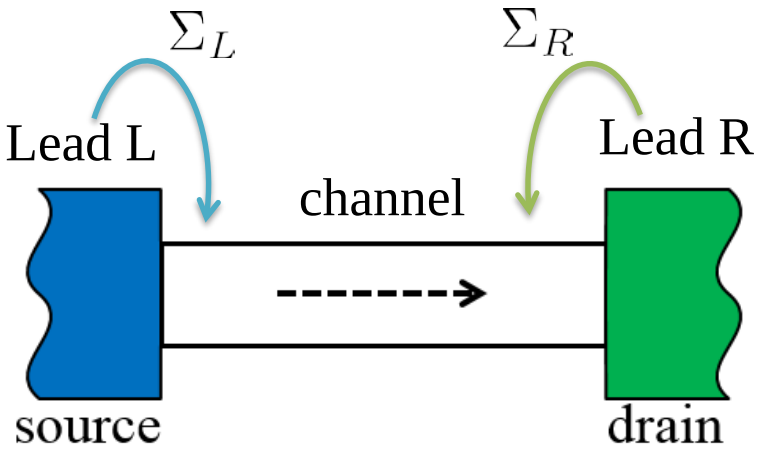
(ii) Green's function of the channel

(iii) equilibrium and non-equilibrium charge densities

(iv) New Hamiltonian is determined by the Poisson equation

Step 3 (Transmission coefficient)

# NEGF for electronic transportation




Surface Green's function of leads

Self-energies of leads $(s = L, R)$

$$\Sigma_s(E) = [ES_{Cs} - H_{Cs}]\, g_s\, [ES_{sC} - H_{sC}]$$

$$\Gamma_s(E) = i\left[\Sigma_s(E) - \Sigma_s^{\dagger}(E)\right]$$

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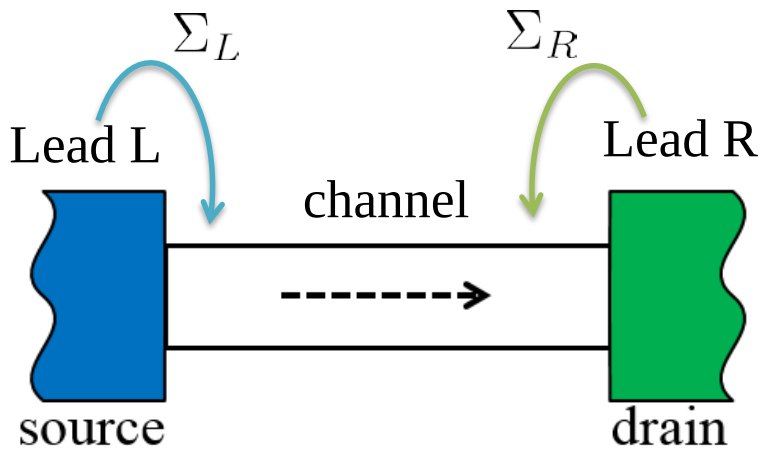
# NEGF for electronic transportation




Kohn-Sham Hamiltonian

$$H(\rho) = T + V_{\text{eff}}(\rho)$$

Green's function

$$G(E) = [ES - H(\rho) - \Sigma_L(E) - \Sigma_R(E)]^{-1}$$

Non-equilibrium density matrix

$$\rho^{\text{neq}} = \rho^{\text{eq}} + \Delta\rho$$

Poisson equation

Step 1 (Lead part)

(i) Electronic structure of the leads

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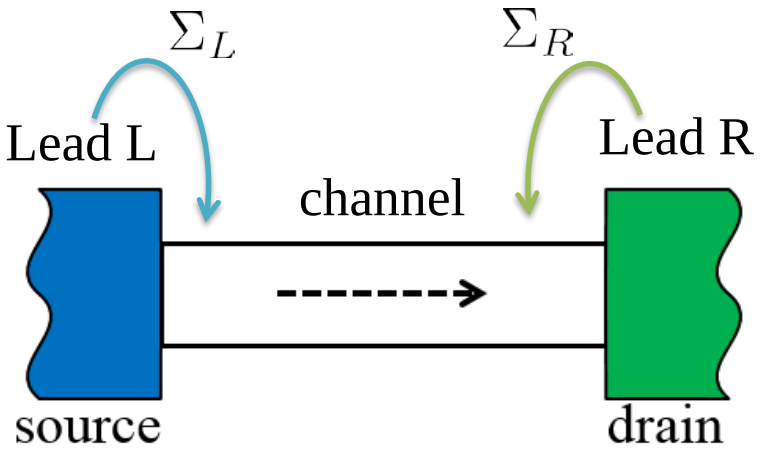
# NEGF for electronic transportation




Transmission coefficient

$$T(E) = \mathrm{Tr}\left[\Gamma_L(E)G(E)\Gamma_R(E)G^{\dagger}(E)\right]$$

Step 1 (Lead part)

(i) Electronic structure of the leads

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Surface Green's function of leads

Poisson equation

Self-energies of leads

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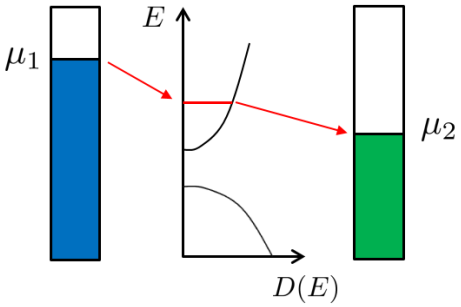
Kohn-Sham Hamiltonian

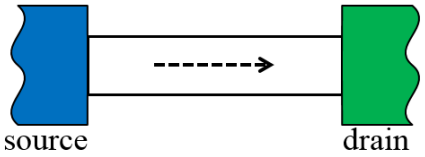
$$H(\rho) = T + V_{\text{eff}}(\rho)$$

Green's function

$$G(E) = [ES - H(\rho) - \Sigma_L(E) - \Sigma_R(E)]^{-1}$$

# NEGF calculation




Non-equilibrium density matrix

$$\rho^{\text{neq}} = \rho^{\text{eq}} + \Delta\rho$$

$$\rho^{\text{eq}} = \rho_+ - \rho_-$$

$$\rho_\pm = \frac{i}{2\pi}\int_{-\infty}^{\infty} dE\, G(E \pm i0^+) f(E-\mu)$$

$$\Delta\rho = \frac{1}{2\pi}\int_{-\infty}^{\infty} dE\, G(E+i0^+)\Gamma_s(E)G(E-i0^+)\Delta f(E)$$

Transmission coefficient

$$T(E) = \text{Tr}\left[\Gamma_L(E)G(E+i0^+)\Gamma_R(E)G(E-i0^+)\right]$$

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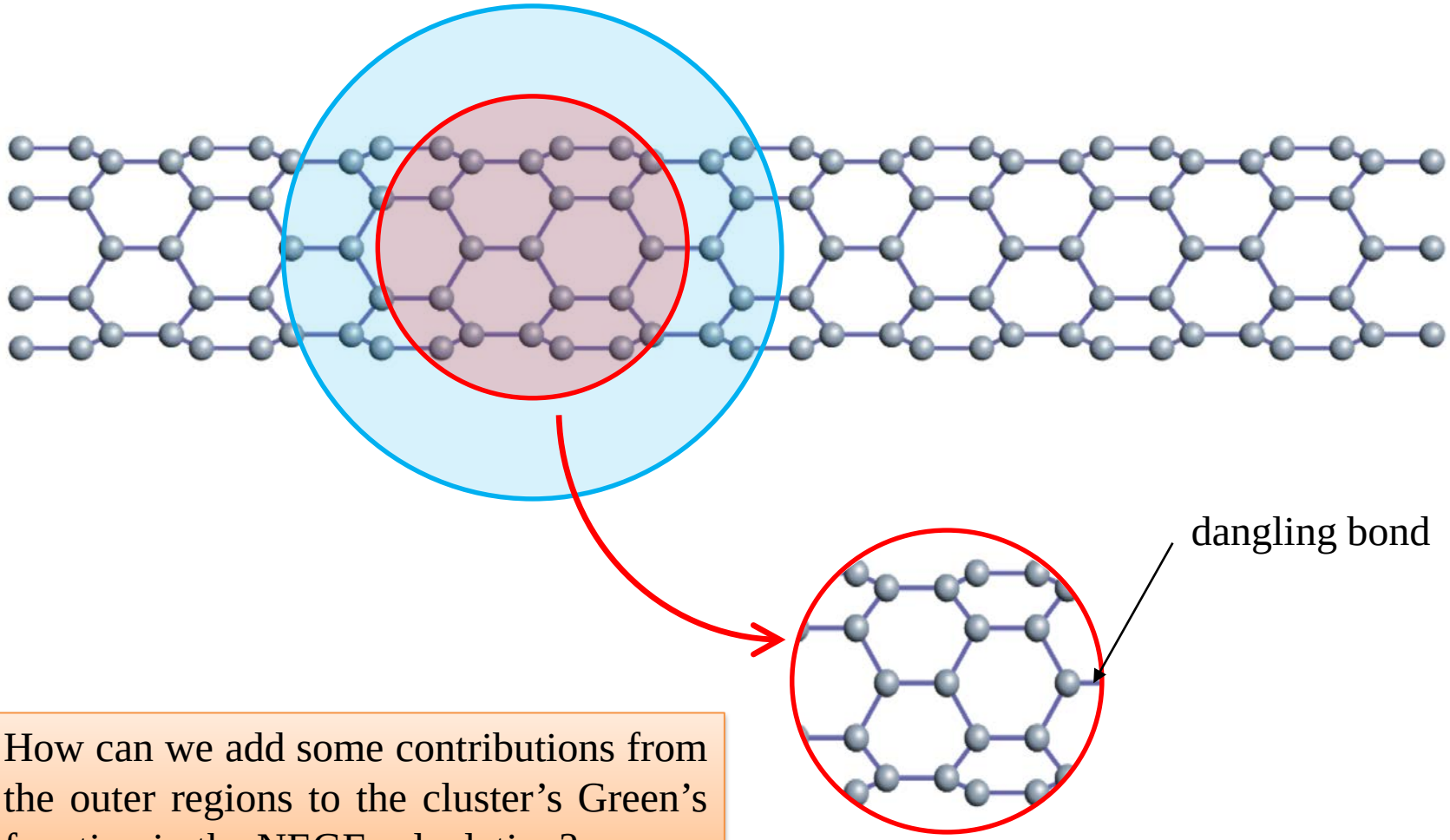
# Divide-conquer method




How can we add some contributions from the outer regions to the cluster's Green's function in the NEGF calculation?

# Separated Green's function (1/3)

$$G(E) = [ES - H(\rho) - \Sigma_L(E) - \Sigma_R(E)]^{-1}$$

$$\Sigma_s(E) = [ES_{Cs} - H_{Cs}]\, g_s\, [ES_{sC} - H_{sC}]$$

outer region

$$G = \begin{pmatrix} A & B \\ C & D \end{pmatrix}^{-1} = \begin{pmatrix} G_A & G_B \\ G_C & G_D \end{pmatrix}$$

inner region

$$\begin{pmatrix} A & B \\ C & D \end{pmatrix}^{-1} = \begin{pmatrix} A^{-1} + A^{-1}B(D - CA^{-1}B)^{-1}CA^{-1} & -A^{-1}B(D - CA^{-1}B)^{-1} \\ -(D - CA^{-1}B)^{-1}CA^{-1} & (D - CA^{-1}B)^{-1} \end{pmatrix}$$

$$G_D = (D - CA^{-1}B)^{-1}$$

When B and C are small enough,

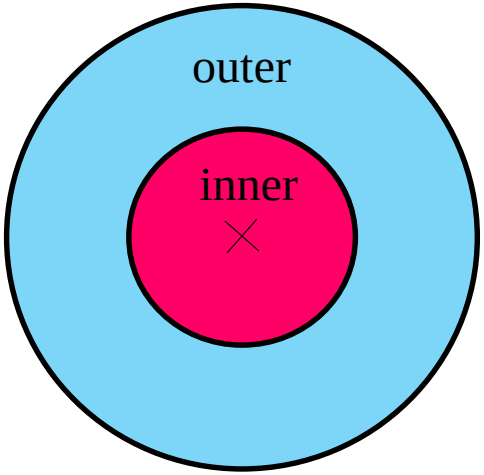
$$A^{-1} \approx G_A$$

$$\therefore G_D \approx (D - C G_A B)^{-1}$$

cluster Hamiltonian

self energy from the outer region

It is difficult to obtain the Green's function of the outer region.



# Separated Green's function (2/3)

$$G(E) = [ES - H(\rho) - \Sigma_L(E) - \Sigma_R(E)]^{-1}$$

$$\Sigma_s(E) = [ES_{Cs} - H_{Cs}]\, g_s\, [ES_{sC} - H_{sC}]$$

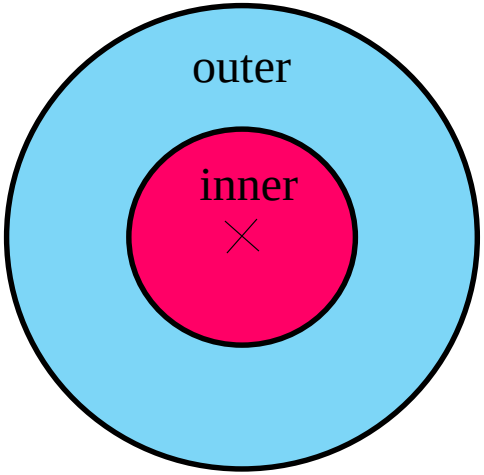
outer region

$$G = \begin{pmatrix} A & B \\ C & D \end{pmatrix}^{-1} = \begin{pmatrix} G_A & G_B \\ G_C & G_D \end{pmatrix}$$

inner region

$$\begin{pmatrix} A & B \\ C & D \end{pmatrix}^{-1} = \begin{pmatrix} A^{-1} + A^{-1}B(D - CA^{-1}B)^{-1}CA^{-1} & -A^{-1}B(D - CA^{-1}B)^{-1} \\ -(D - CA^{-1}B)^{-1}CA^{-1} & (D - CA^{-1}B)^{-1} \end{pmatrix}$$

$$G_D = (D - CA^{-1}B)^{-1}$$




When B and C are small enough,

$$A^{-1} \approx G_A \approx \tilde{G}_A$$

$\tilde{G}_A$ : Green's function obtained by the previous SCF step

$$\therefore G_D \approx (\underline{D} - \underline{C\tilde{G}_A B})^{-1}$$

cluster Hamiltonian — self energy

The clustered Green's function can be improved by using $\tilde{G}_A$ .

# Separated Green's function (3/3)

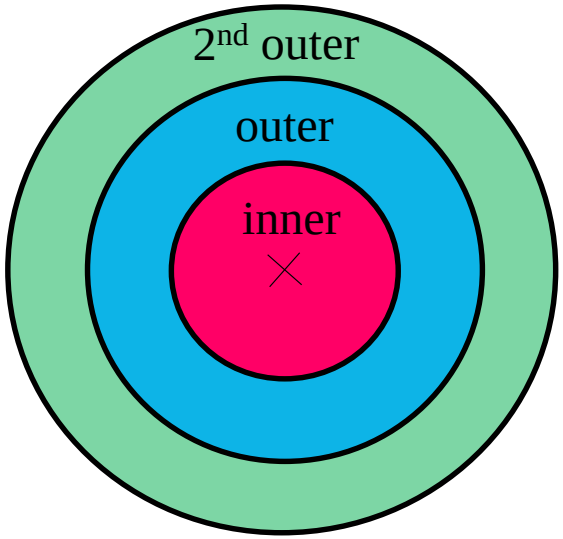
$$G_D = (D - CA^{-1}B)^{-1}$$

$$G = \begin{pmatrix} A & B_{11} & B_{12} \\ C_{11} & D_{11} & D_{12} \\ C_{21} & D_{21} & D_{22} \end{pmatrix}^{-1}$$

2nd outer region

outer region

inner region




$$G_{D_{22}} = \left[ D_{22} - \begin{pmatrix} C_{21} & D_{21} \end{pmatrix} \begin{pmatrix} A & B_{11} \\ C_{11} & D_{11} \end{pmatrix}^{-1} \begin{pmatrix} B_{12} \\ D_{12} \end{pmatrix} \right]^{-1}$$

$$\approx \left[ D_{22} - D_{21} \left( D_{11} - C_{11}A^{-1}B_{11} \right)^{-1} D_{12} \right]^{-1}$$

$$\because B_{12} \approx 0, \quad C_{21} \approx 0$$

$$G_{D_{11}} \approx \left( D_{11} - C_{11}A^{-1}B_{11} - D_{12}D_{22}^{-1}D_{21} \right)^{-1}$$

effect from the inner region to the outer region

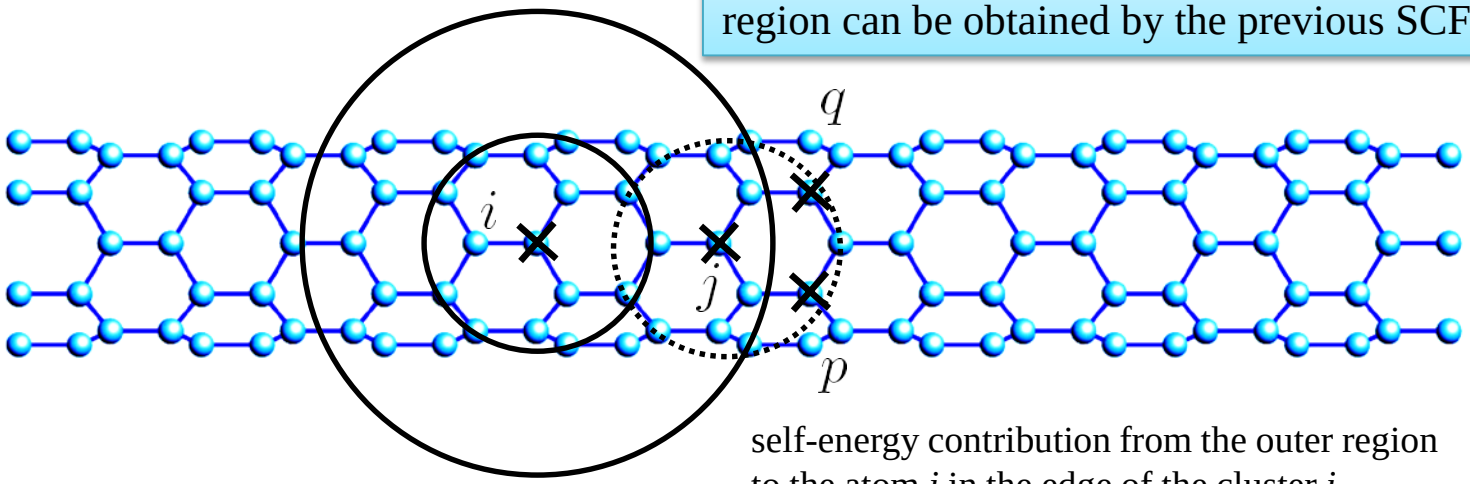
$$G'_{D_{11}} \equiv \left( D_{11} - C_{11}A^{-1}B_{11} \right)^{-1}$$

$$G_{D_{22}} = \left( D_{22} - D_{21}G'_{D_{11}}D_{12} \right)^{-1} \rightarrow \left( D_{22} - D_{21}\tilde{G}_{D_{11}}D_{12} \right)^{-1}$$

This approximated local Green's function includes both outer regions effect.

# Implementation to DC-NEGF

The GF in the truncated cluster can be calculated if the GF in the outer region is known. Approximate GF in the outer region can be obtained by the previous SCF step calculation.




self-energy contribution from the outer region to the atom *j* in the edge of the cluster *i*

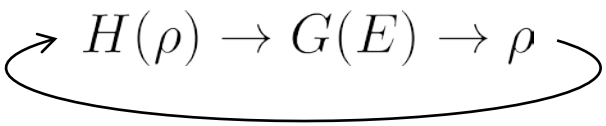
$$\Sigma_j^{(i)}(E) = \sum_{p,q} \left[ES_{jp} - H_{jp}\right] \tilde{G}_{pq} \left[ES_{qj} - H_{qj}\right]$$

$$G^{(i)}(E) = \left[ ES^{(i)} - H^{(i)}(\rho) - \Sigma_L^{(i)}(E) - \Sigma_R^{(i)}(E) - \sum_j \Sigma_j^{(i)}(E) \right]^{-1}$$

The clusters' Green's functions can include the contribution from the outer region by adding the correction by the self energy term. It improves the accuracy of the clusters' Green's functions and a convergence of the divide-conquer NEGF calculation.

# Algorisms for NEGF and DC-NEGF

## ordinary NEGF




```
do scf
   solve Poisson equation
   do E
      construct InvG=ES-H-Σ_L-Σ_R
      calculate G(E)
      calculate ρ^eq(E)
      calculate G^<(E)
      calculate Δρ(E)
   end do
end do
```

MPI parallelization about E

## DC-NEGF

The computational cost of the DC-NEGF calculation scales only linearly.

```
do scf
   solve Poisson equation
   do E
      construct InvG=ES-H-Σ_L-Σ_R
      do site i
         construct InvG^(i)
         construct InvG^(i)-Σ^(i)
         calculate G^(i)(E)
         calculate ρ^eq(i)(E)
      end do
      construct G(E) and ρ^eq(E)
      calculate G^<(E)
      calculate Δρ(E)
   end do
end do
```

MPI parallelization about E and clusters

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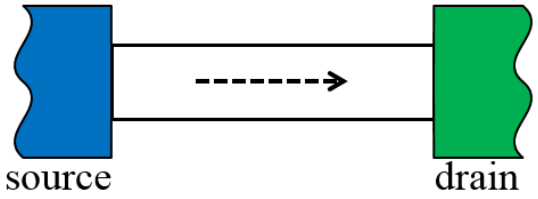
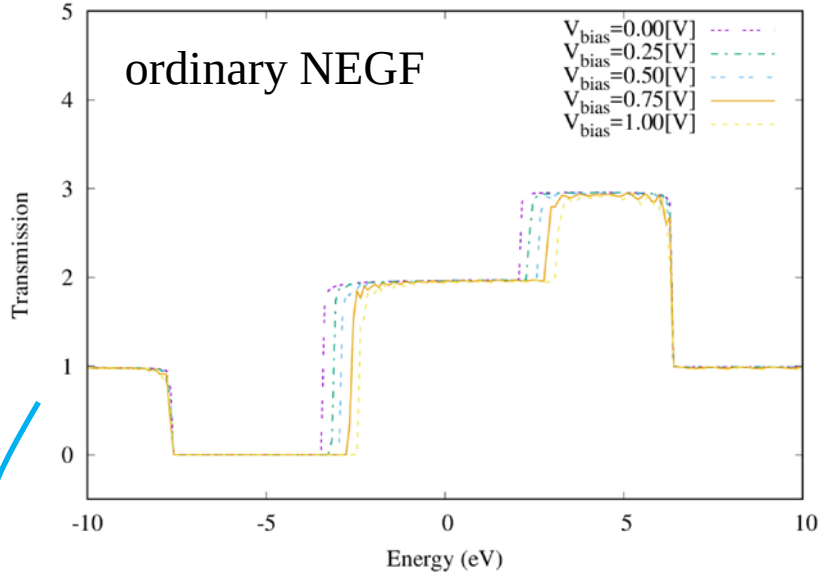
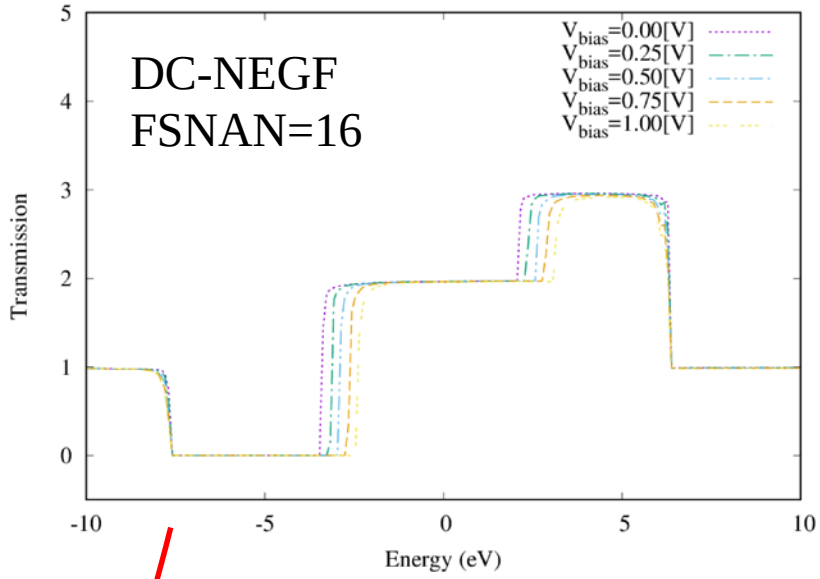
# Computational details

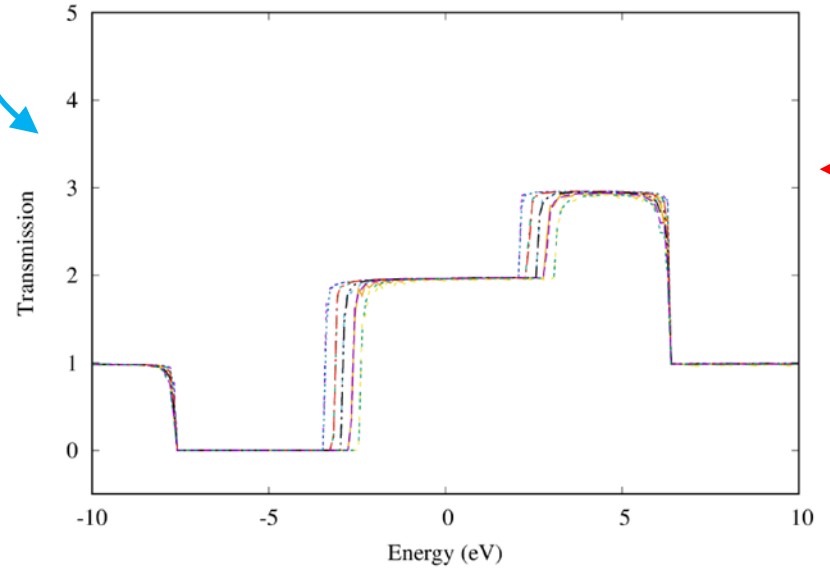
- Program code
  - OpenMX (http://www.openmx-square.org/)
- Method: NEGF and DC-NEGF
- Carbon chain ($C_{36}$)
  - LDA
  - basis set : C5.0-*s*1*p*1
  - number of energy poles : 100
  - T=600[K]
- (6,0) zigzag carbon nanotube ($C_{192}$)
  - LDA
  - basis set : C5.0-*s*2*p*1
  - number of energy poles : 100
  - T=300[K]

# Transmission, carbon chain ($C_{36}$)



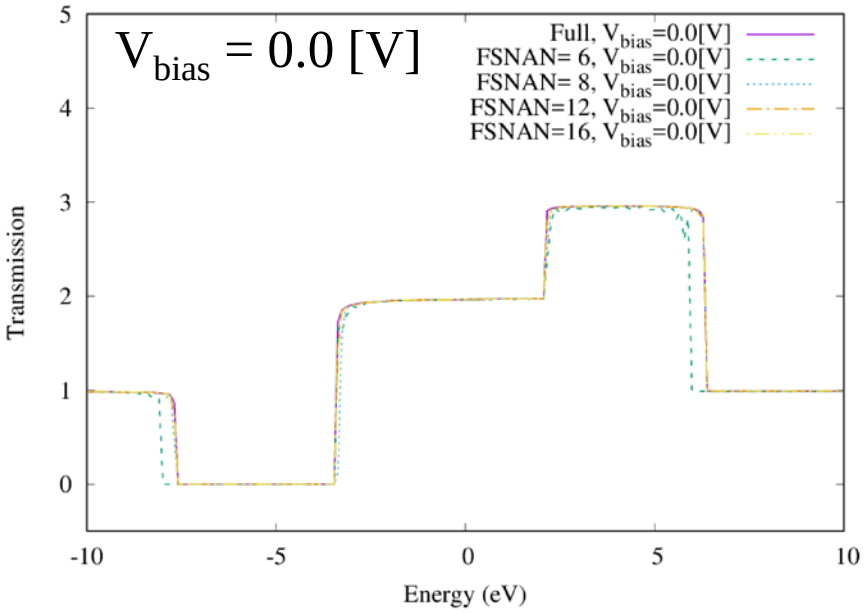



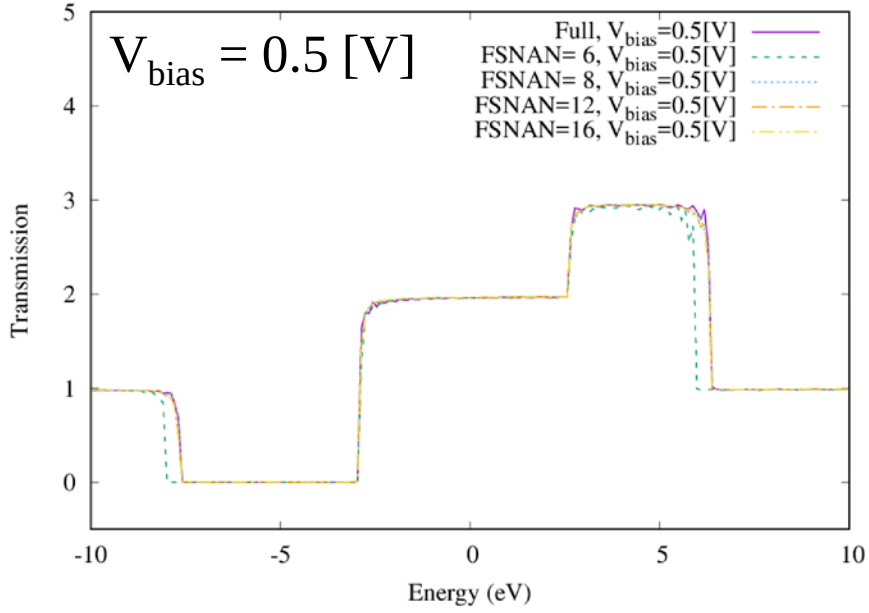




FSNAN: the number of the atoms in the truncated clusters

Good agreement!

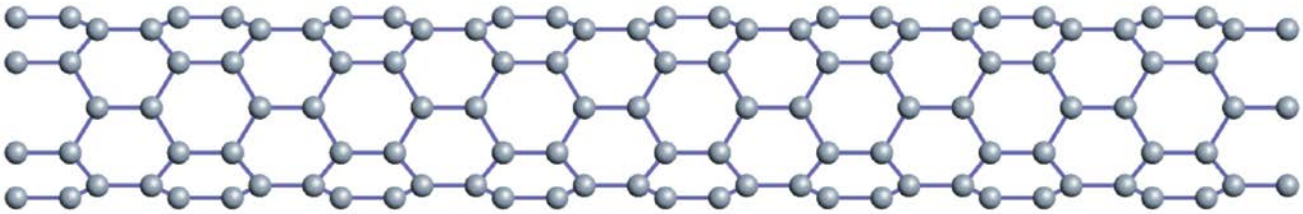
# Transmission, carbon chain ($C_{36}$) truncated cluster size dependency

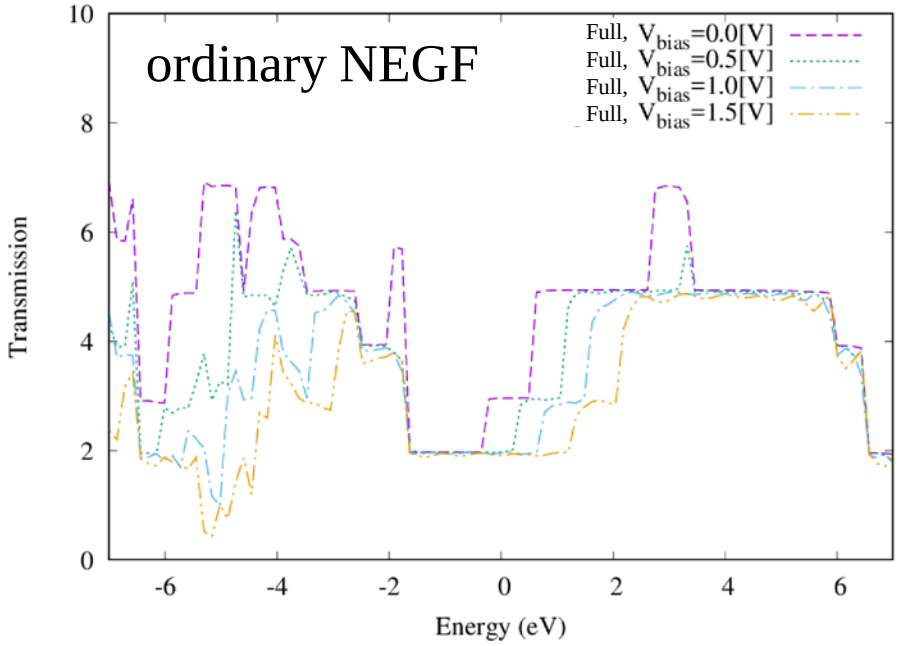


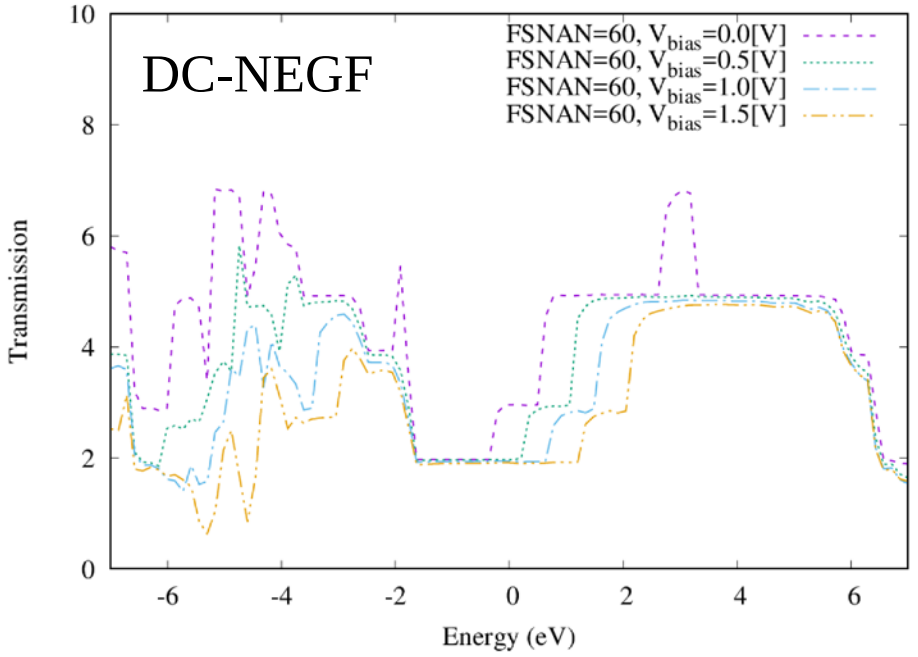




Better agreement with the original NEGF calculation result is obtained by using the larger truncated cluster size.

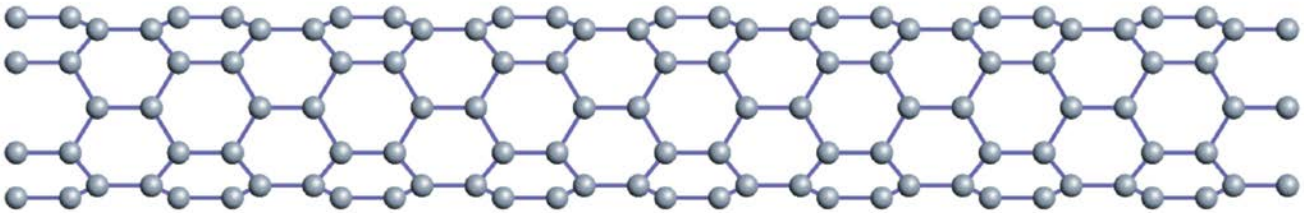
# Transmission,
# (6,0) zigzag carbon nanotube ($C_{192}$)

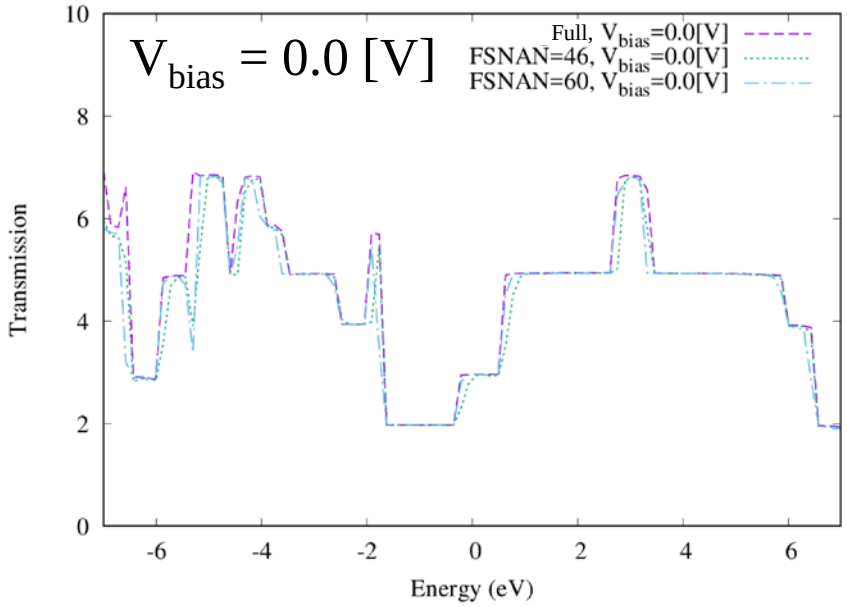


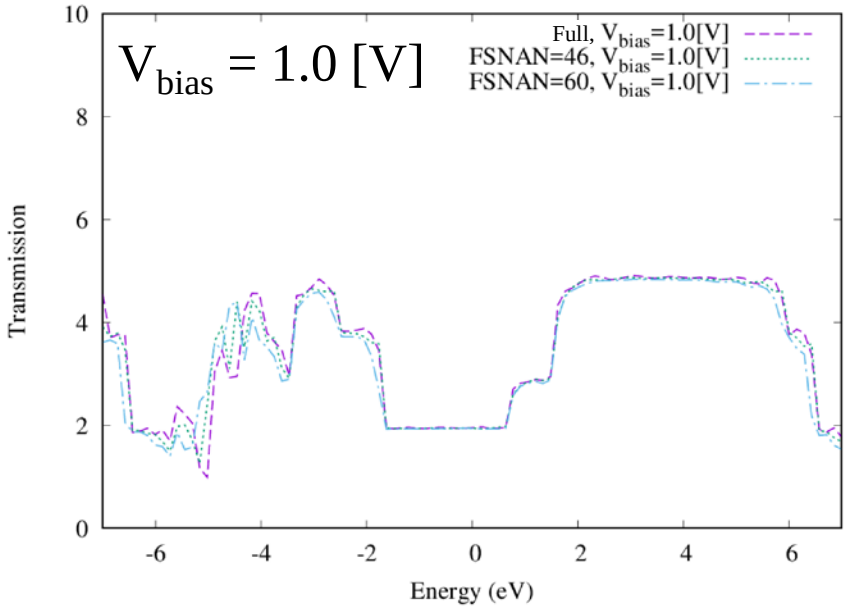


# Transmission, (6,0) zigzag carbon nanotube ($C_{192}$), truncated cluster size dependency





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# Conclusion

- We have proposed a linear scaling NEGF method based on a divide-conquer (DC) approach with a correction by self-energy terms, whose computational cost scales only linearly.

- It can be confirmed that our implementation gives sufficient accuracy to transmission calculations.

- It allows us to extend the applicability of the NEGF to realistic large scale systems.