MS-DFT: Quantum Transport from a Multi-Space Excitation Viewpoint

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IWCN 2023 Barcelona, Spain
Monday, June 12, 2023

KAIST

EE

Outline

I. Background information
   - DFT-NEGF: Difficulties → Beyond DFT-NEGF?
   - DFT vs NEGF
   - NEGF ≠ Landauer

II. MS-DFT: development & its applications

III. Summary

Beyond DFT: Equilibrium → Non-Equilibrium

❑ **Density Functional Theory (DFT)** — **Energy, structure, …** — **@ Equilibrium**

- VASP
- SIESTA
- Gaussian

etc. etc.

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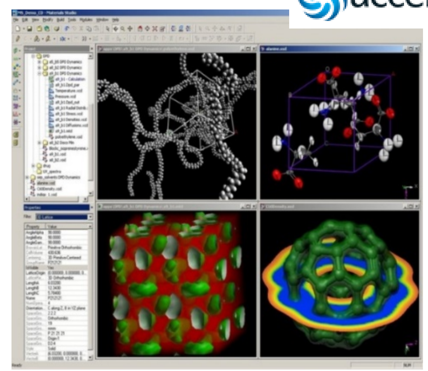

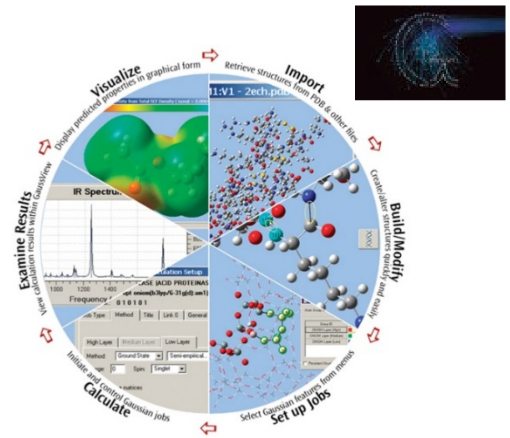

❑ **GW+BSE & time-dependent DFT** — **Optical excitation, …** — **@ Non-equilibrium**

❑ **Non-Equilibrium Green's function (NEGF)** — **Quantum transport, …** — **@ Non-equilibrium**

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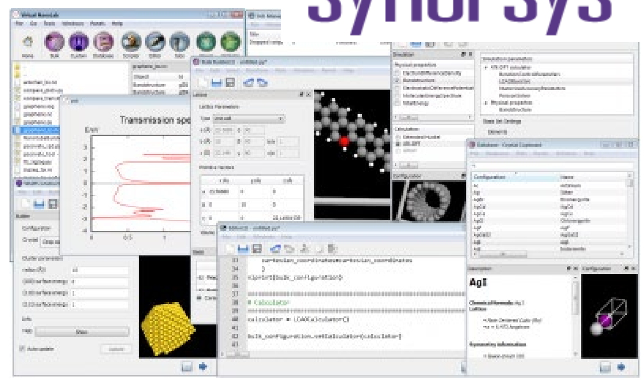

- TranSIESTA
- QuantumATK

etc.

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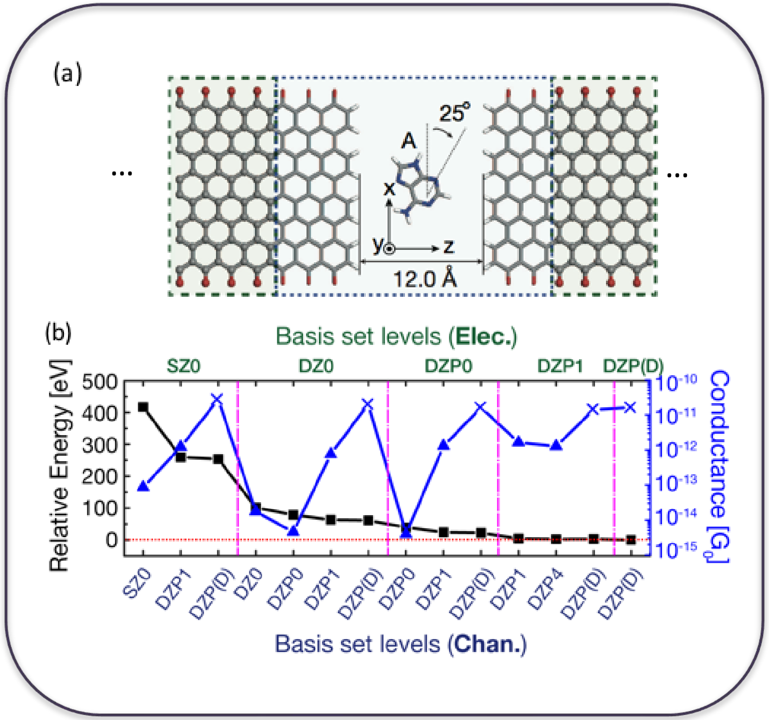
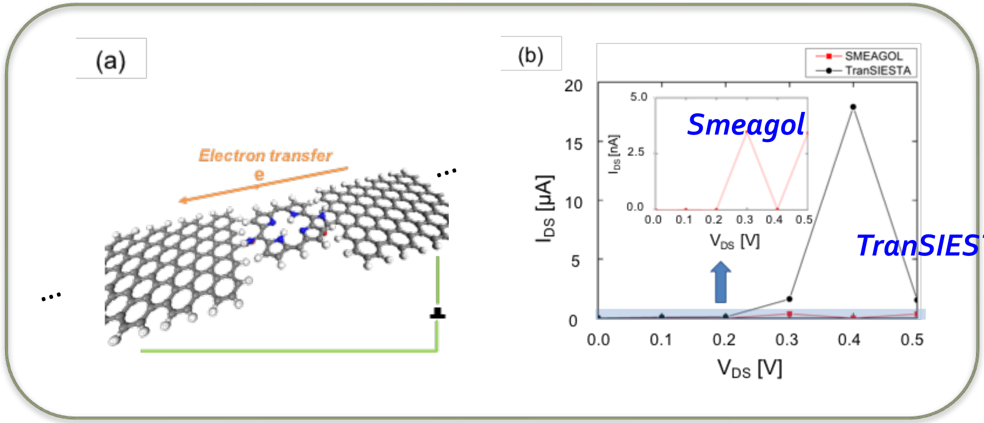
Difficulties with NEGF (beyond-DFT methods in general)

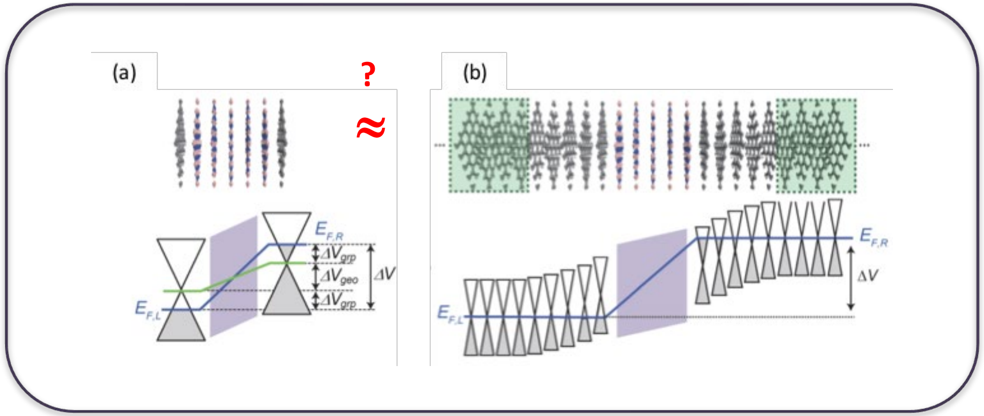
Various difficulties from NEGF



Nonvariational nature of "Landauer" current ($V_b = 0$ V)



Inequivalence between different codes ($V_b \neq 0$ V)



Restrictions from the requirement of semi-infinite electrodes ($V_b \neq 0$ V)

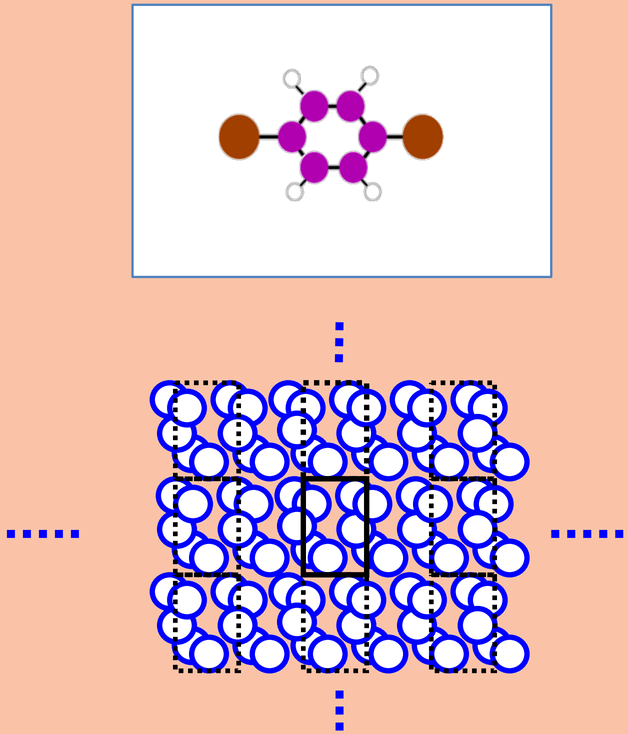
DFT vs NEGF: Closed vs Open B.C.

DFT (Equilibrium)

Closed or Periodic B. C.

$H\psi_i = \varepsilon_i \psi_i$

$f_{FD}(E - \mu)$

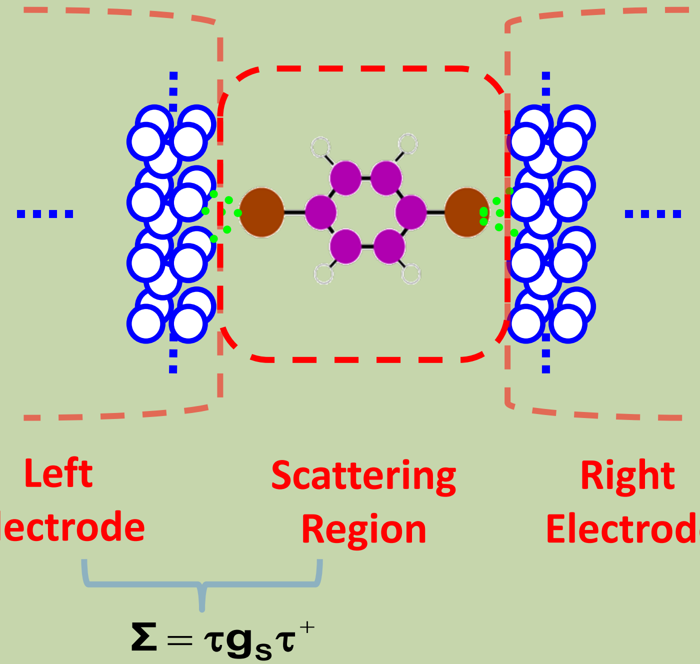


NEGF (Non-equilibrium)

Open B. C.

$G^R = (E1 - H - \Sigma_1 - \Sigma_2)^{-1}$

$G^n(E) \approx f_1 A_1(E) + f_2 A_2(E)$



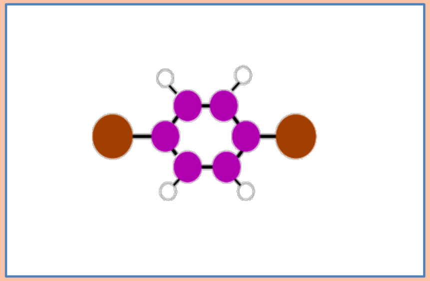
DFT vs NEGF: Closed vs Open B.C.

DFT (Equilibrium)

Closed or Periodic B. C.

$$H\psi_i = \varepsilon_i \psi_i$$

$$f_{FD}(E-\mu)$$



☺ **High-reliability of simulations!!**

$$E[\chi] = \frac{\langle \chi | H | \chi \rangle}{\langle \chi | \chi \rangle} \rightarrow E[\chi] \geq E_{GS} = \langle \psi_{GS} | H | \psi_{GS} \rangle$$

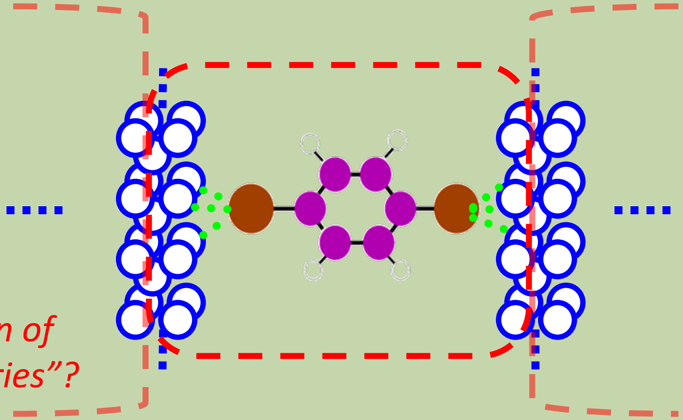
- Total energy ← Variational principle

NEGF (Non-equilibrium)

Open B. C.

$$G^R = (E1 - H - \Sigma_1 - \Sigma_2)^{-1}$$

$$G^n(E) \approx f_1 A_1(E) + f_2 A_2(E)$$



☹ **Ambiguities??**

$$I(V) \approx \frac{e}{h} \int dE\, Tr(\mathbf{\Gamma_1 G \Gamma_2 G^+})\, [f_1 - f_2]$$

- Current: Non-variational quantity

Remind: NEGF assumptions

Valid for: time-dependent Schrodinger eq. & closed quantum system

- Retarded Green's function (~ DOS):

$$\mathbf{G}^R(E) = [(E + i0^+)\mathbf{1} - \mathbf{H}]^{-1}$$

→ Spectral function (~"DOS")

$$\mathbf{A}(E) = i[\mathbf{G}(E) - \mathbf{G}^+(E)]$$

- Correlation function (~ density):

$$\underbrace{\mathbf{G}^n}_{\psi\psi^+} = \mathbf{G}^R \underbrace{\mathbf{\Sigma}^{in}}_{ss^+} \mathbf{G}^A$$

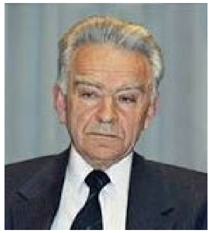
"Keldysh eq."

→ Density matrix

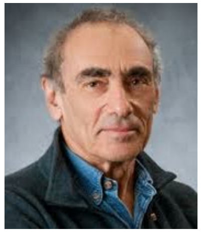
$$\mathbf{D} = \frac{1}{2\pi}\int_{-\infty}^{+\infty} dE\,\mathbf{G}^{\mathrm{n}}(E)$$

or Density

$$n(\vec{r}) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} dE\,\mathbf{G}^{\mathrm{n}}(\vec{r}, E)$$



Leonid Keldysh
(1931~2016)



Gordon Baym
(1935~)

Leo Kadanoff
(1937~2015)

- *Closed quantum systems*
- *Initial global equilibrium*
- *Adiabatic approach to non-equilibrium state*

"Electronic Transport in Mesoscopic Systems"
by S. Datta (1997)
"Electrical Transport in Nanoscale Systems"
by M. Di Ventra (2008)

DFT-NEGF: NEGF + Landauer (Landauer ≠ NEGF!)

$$i\hbar\frac{\partial\psi(t)}{\partial t} = H(t)\psi(t) + \int_0^t dt'\Sigma(t,t')\psi(t') + s(t)$$

- Self-energy:

$$\mathbf{G}^R(E) = [E\mathbb{I} - \mathbf{H} - \boldsymbol{\Sigma}_1(E) - \boldsymbol{\Sigma}_2(E)]^{-1}$$

- "Landauer condition":

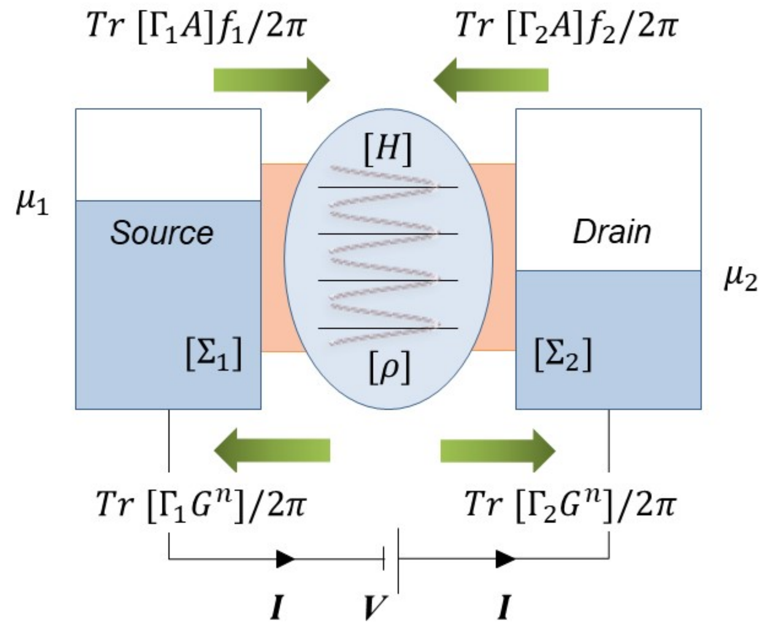
$$\boldsymbol{\Sigma}^{in} \approx \boldsymbol{\Gamma}_1 f_1 + \boldsymbol{\Gamma}_2 f_2$$

$$\rightarrow n(\vec{r}) \approx \frac{1}{2\pi}\int_{-\infty}^{+\infty} dE[f_1\mathbf{A}_1 + f_2\mathbf{A}_2]$$

- Terminal current:

$$I = \frac{e}{h}\int dE\,\{Tr[\boldsymbol{\Gamma}_\alpha\mathbf{A}]f_\alpha - Tr[\boldsymbol{\Gamma}_\alpha\mathbf{G}^n]\}$$

$$\approx \frac{e}{h}\int dE\,\underbrace{Tr(\boldsymbol{\Gamma}_1\mathbf{G}\boldsymbol{\Gamma}_2\mathbf{G}^+)}_{\text{Transmission}}\,[f_1(E) - f_2(E)]$$

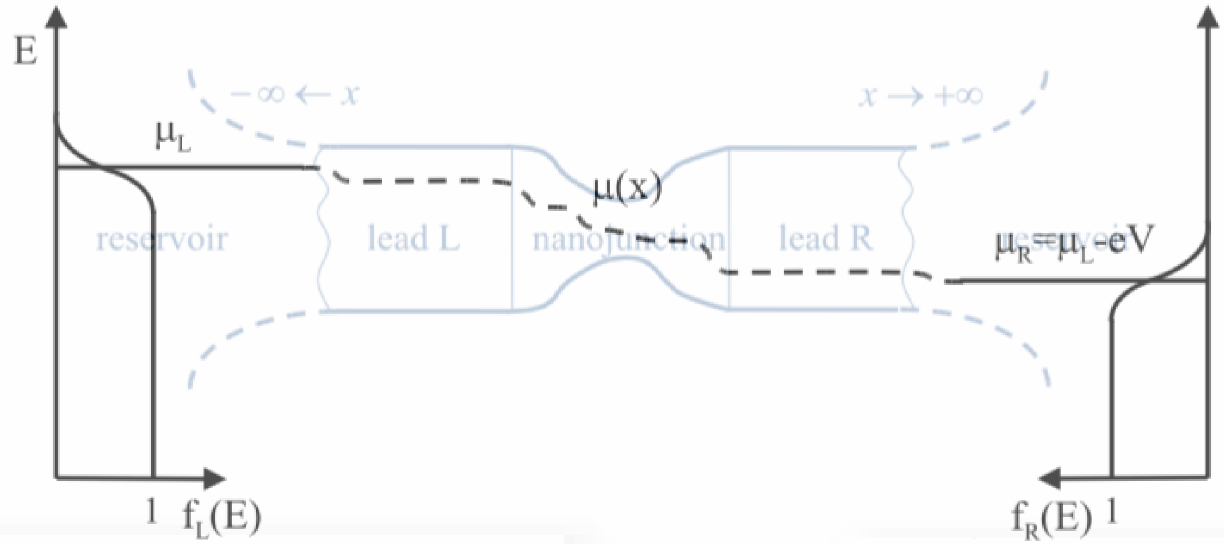


- *Time-dependent → Steady state transport*
- *Closed → Open quantum system via BC*

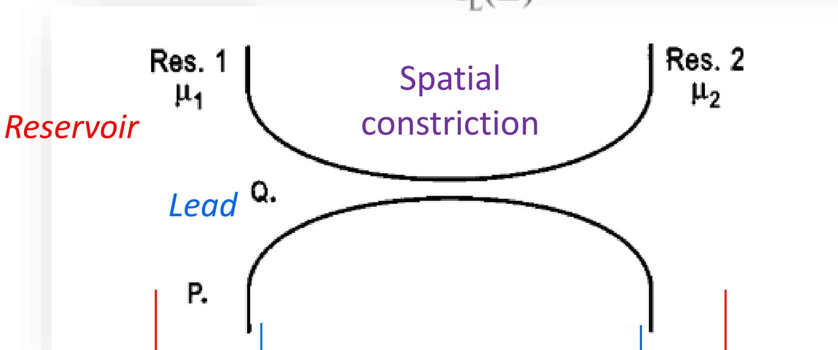
"Electronic Transport in Mesoscopic Systems" by S. Datta (1997)
"Electrical Transport in Nanoscale Systems" by M. Di Ventra (2008)

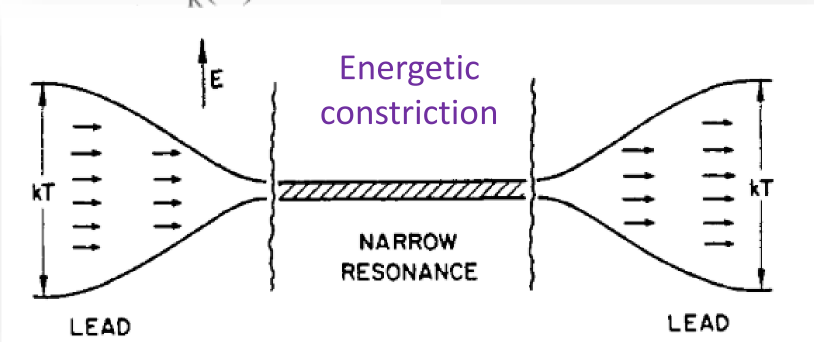
Landauer “picture” for quantum transport

“… it is a viewpoint, not a specific equation.”



Rolf William Landauer
(1927~1999)





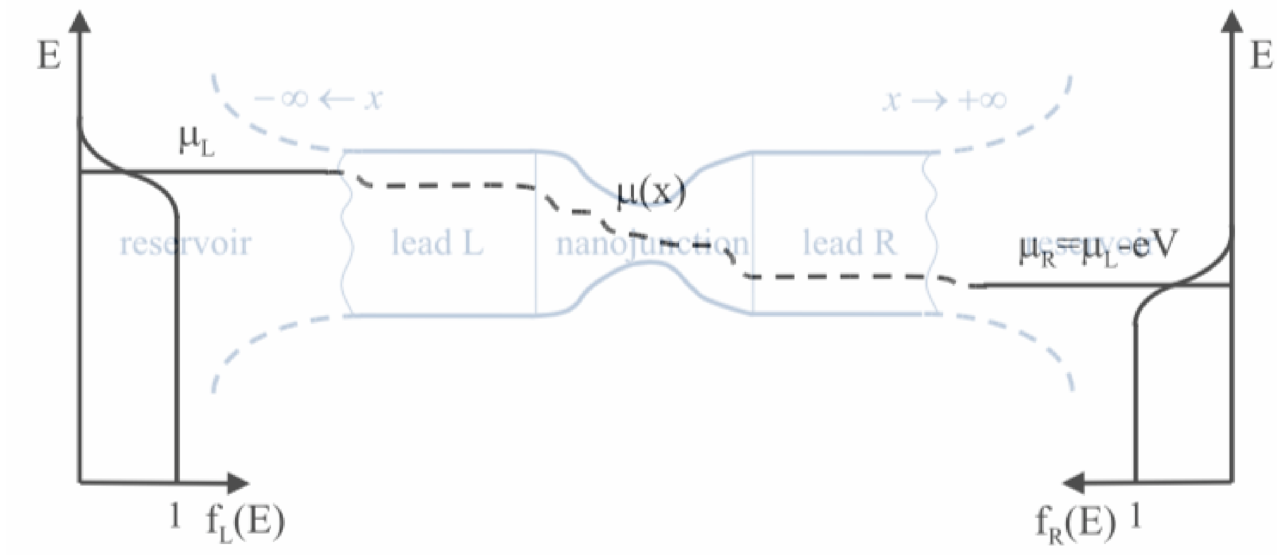
$$G_B = \frac{2e^2}{h}\frac{T}{1-T}$$

$$G_B = \frac{2e^2}{h}T$$

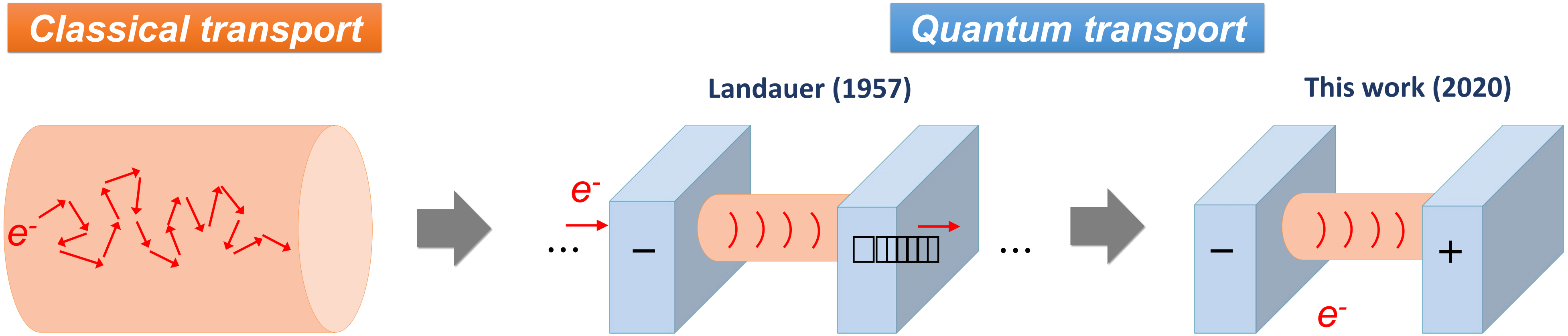
R. Landauer, *Z. Phys. B* **68**, 217 (1987)
R. Landauer, *J. Phys. Condens. Matter* **43**, 8099 (1989)
R. Landauer, *Phys. Scr.* **T42**, 110 (1992)
Y. Imry & R. Landauer, *Rev.Mod. Phys.* **71**, S306 (1999)

Objective of this work

Q. Beyond DFT-NEGF? ← Alternative to the Landuer picture?



Rolf William Landauer
(1927~1999)



Outline

I. Background information: DFT, NEGF, & Landauer

II. MS-DFT: development & its applications

- Formulation → Total energy
- Voltage drop: Quasi-Fermi level splitting & Landauer resistivity dipole
- Graphene vertical vdW tunneling transistor & NDR
- *Electric enthalpy & Interfacial water*

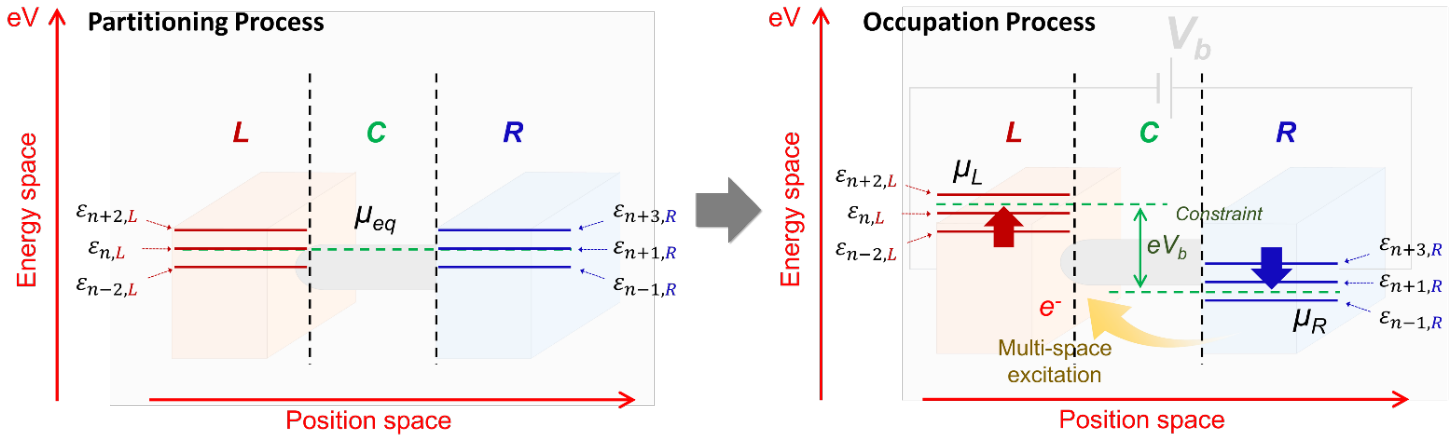
III. Summary

Alternative to Landauer & DFT-NEGF?

Multi-Space constrained-search DFT (MS-DFT)

*1. Steady-state **quantum transport***
*= Time-independent **multi-space optical excitation***

cf. Landauer viewpoint



*2. Micro-canonical → **Variational** (constrained-search) DFT quantum transport calculation*

cf. DFT-NEGF

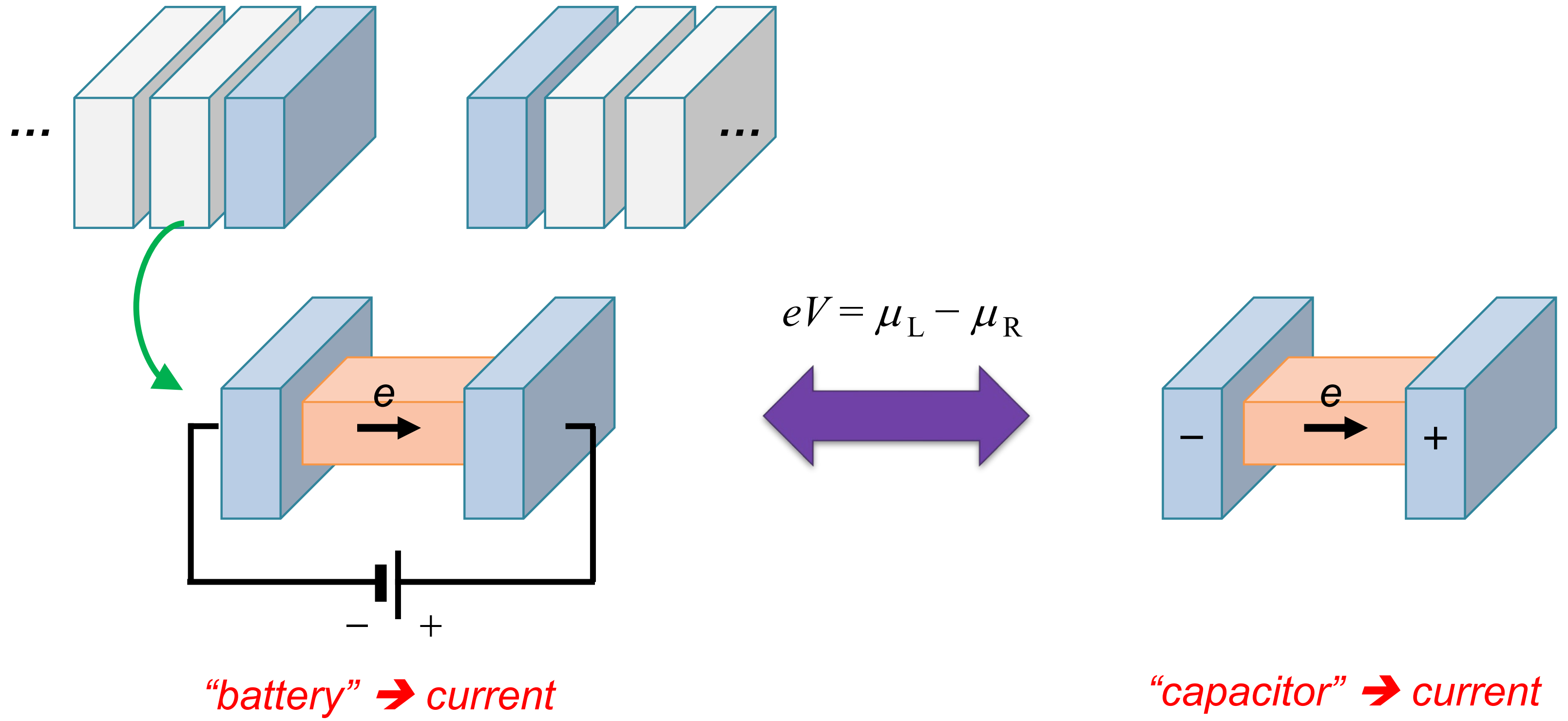
- H.S. Kim & YHK, arXiv [cond-mat.mes-hall], 1808.03608 (2018)
- J. Lee, H. Yeo, & YHK, PNAS **117**, 10142 (2020)
- T.H. Kim, J. Lee, R.-G. Lee, & YHK, Adv. Sci. **7**, 2001038 (2020)

Multi-Space constrained-search DFT: Formulation

Quantum transport = Multi-space (space-discriminating) excitation
→ Variational DFT calculation of steady-state current

Step 1. Viewpoint: Grand-canonical ("Landauer") ⇔ Micro-canonical

Di Ventra & Todorov, J. Phys. Cond. Matt. ***16****, 8025 (2004).*

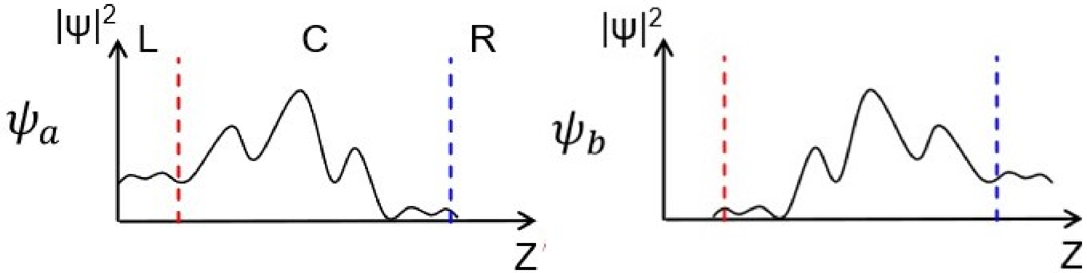


MS-DFT: Formulation – Step 2

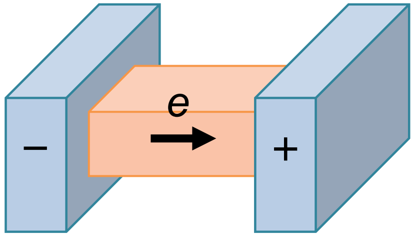
Quantum transport* = *Multi-space (space-discriminating) excitation
→ Variational DFT calculation of steady-state current

Step 2. Assign Ψ to *L*, *C*, & *R* regions

"locality" or "near-sightness" in C (semi-conductors)
(W. Kohn)



$$\psi_i(\vec{r}) \in \begin{cases} \psi_i^{\mathrm{L}} \text{ if } \int_{\mathrm{L}} |\psi_i(\vec{r})|^2 d^3r > \int_{\mathrm{C/R}} |\psi_i(\vec{r})|^2 d^3r, \\ \psi_i^{\mathrm{C}} \text{ if } \int_{\mathrm{C}} |\psi_i(\vec{r})|^2 d^3r > \int_{\mathrm{L/R}} |\psi_i(\vec{r})|^2 d^3r, \\ \psi_i^{\mathrm{R}} \text{ if } \int_{\mathrm{R}} |\psi_i(\vec{r})|^2 d^3r > \int_{\mathrm{L/C}} |\psi_i(\vec{r})|^2 d^3r \end{cases}$$



- $V = 0 : \rho_0(\vec{r}) = \rho_0^L(\vec{r}) + \rho_0^C(\vec{r}) + \rho_0^R(\vec{r})$
- $V \neq 0: \rho_k(\vec{r}) = \rho_k^L(\vec{r}) + \rho_k^C(\vec{r}) + \rho_k^R(\vec{r})$

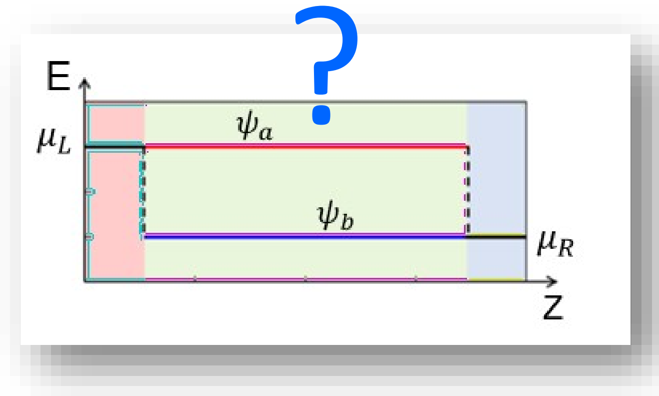
MS-DFT: Formulation – Step 3

Quantum transport = Multi-space (space-discriminating) excitation
→ Variational DFT calculation of steady-state current

Step 3. quantum transport ⇔ Multi-electrode *(drain → source)* excitation

cf. Variational time-independent excited-state DFT

- M. Levy & Á. Nagy, *Phys. Rev. Lett.* **83,** 4361 (1999).
- A. Görling, *Phys. Rev. A* **59,** 3359 (1999).



For the "excited" state k;

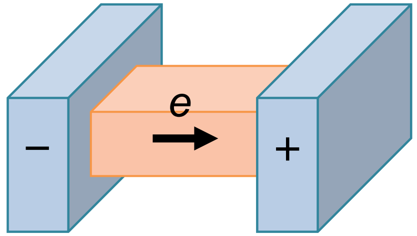
$$E_k = \min_\rho \left\{ \int v(\vec{r})\,\rho(\vec{r}) d^3\vec{r} + F\left[\rho_k^L, \rho_k^C, \rho_k^R, \rho_0\right] \right\}$$
$$= \int v(\vec{r})\,\rho(\vec{r}) d^3\vec{r} + F[\rho_k, \rho_0]$$

orthogonal

with

$$F[\rho_k, \rho_0] = \min_{\Psi^{L/C/R} \to \rho_k} \langle \Psi_{L/C/R} | \hat{T} + \hat{V}_{ee} | \Psi_{L/C/R} \rangle$$

→ Constrained Search (constraint: $eV = \mu_R - \mu_L$)



$$\rho_k(\vec{r}) = \rho_k^L(\vec{r}) + \rho_k^C(\vec{r}) + \rho_k^R(\vec{r})$$

MS-DFT: Formulation – Step 4

Quantum transport = Multi-space (space-discriminating) excitation
→ Variational DFT calculation of steady-state current

Step 4. Transmission & current as post-processing processes

- Semi-infinite electrodes (recover Landauer):

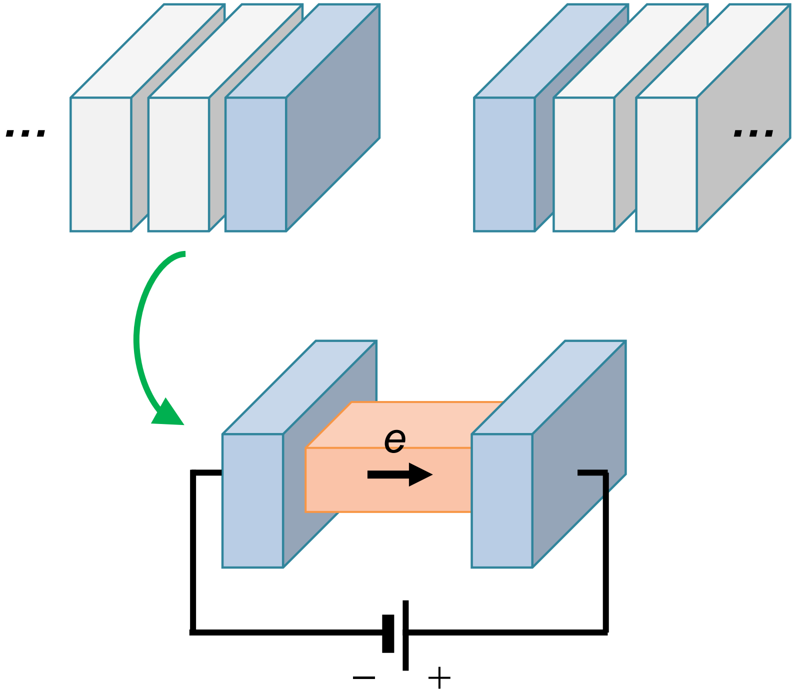
$$T(E;V) = Tr\left[\Gamma_L G \Gamma_R G^\dagger\right]$$

- Finite electrodes:

$$T(E;V) = Tr\left[\mathrm{A}_L M \mathrm{A}_R M^\dagger\right] \quad \text{with} \quad M = \tau_L^+ G \tau_R$$

- I-V:

$$I(V) = \frac{e}{h}\int_{-\infty}^{\infty} dE \;\; T(E;V)\,[f_1(E) - f_2(E)]$$



MS-DFT: Kohn-Sham scheme

N.B. "Current" is not our simulation target any more.
→ Instead, minimizing "energy" within the "constraint $eV = \mu_1 - \mu_2$"

0. Applied bias as a constraint: $eV = \mu_1 - \mu_2$
1. Assign ψ_i to L/C/R (multi-space) regions
2. Minimize energy functional via constrained search :

$$E_k = \min_\rho \left\{ \int v(\vec{r})\, \rho(\vec{r}) d^3\vec{r} + F\left[\rho_k^L, \rho_k^C, \rho_k^R, \rho_0\right] \right\} \quad \text{(total energy)}$$

$$F[\rho_k, \rho_0] = \min_{\Psi^{L/C/R} \to \rho_k} \langle \Psi_{L/C/R} | \hat{T} + \hat{V}_{ee} | \Psi_{L/C/R} \rangle \quad \text{(universal functional)}$$

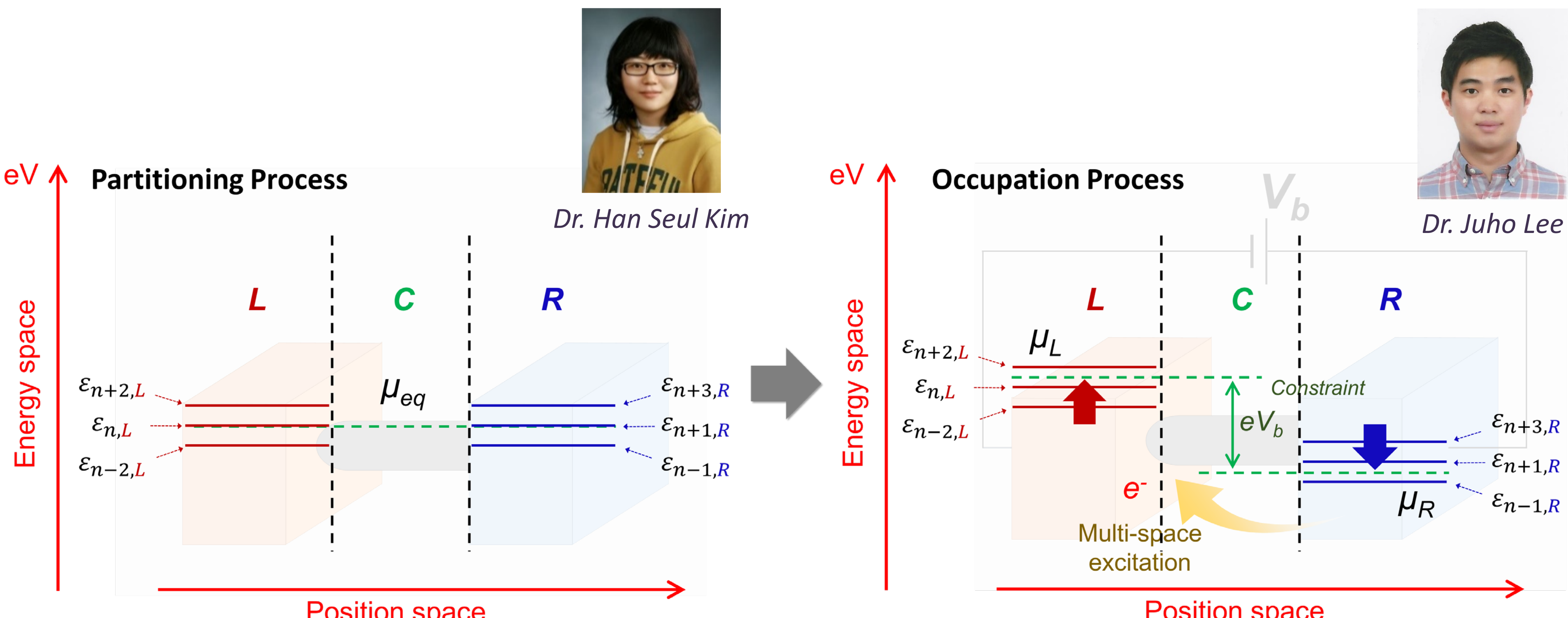
⇒ Solve (non-equilibrium) Kohn-Sham (KS) equations

$$\left[\hat{h}_{KS}^0 + \Delta v_{Hxc}(\vec{r})\right] \psi_i(\vec{r}) = \varepsilon_i\, \psi_i(\vec{r})$$

MS-DFT: Summary & Implementation

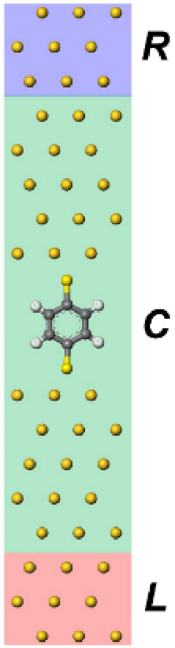
Quantum transport = Multi-space (space discriminating) excitation

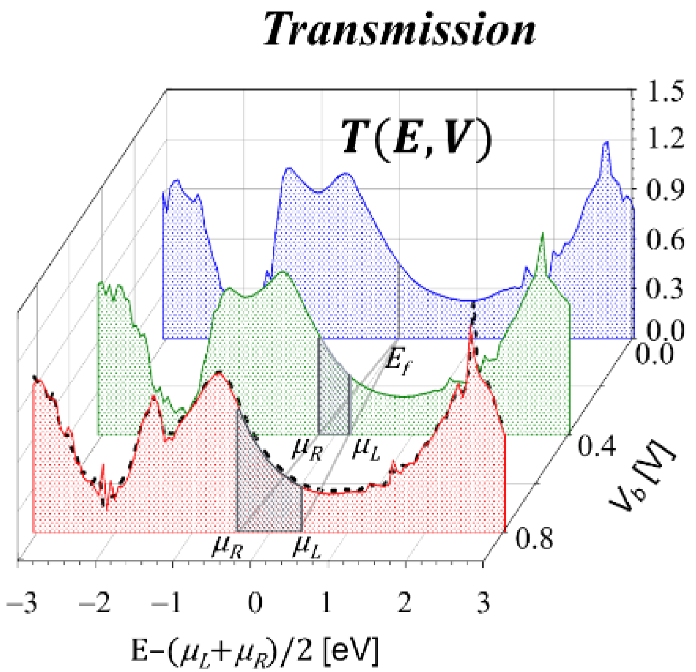
→ Variational constrained-search DFT calculation of quantum transport

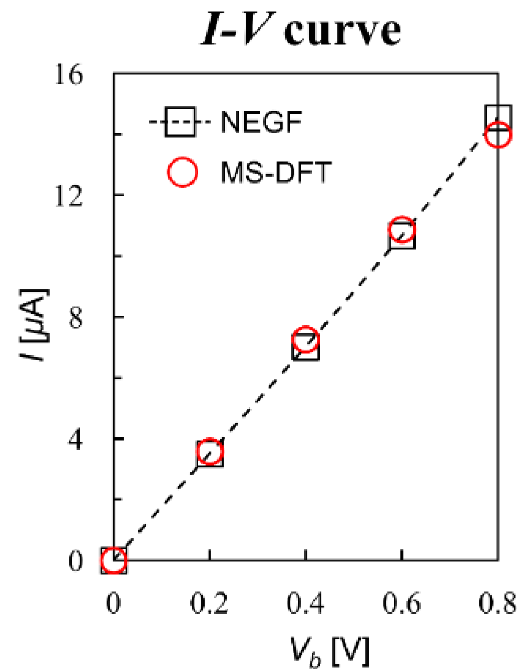


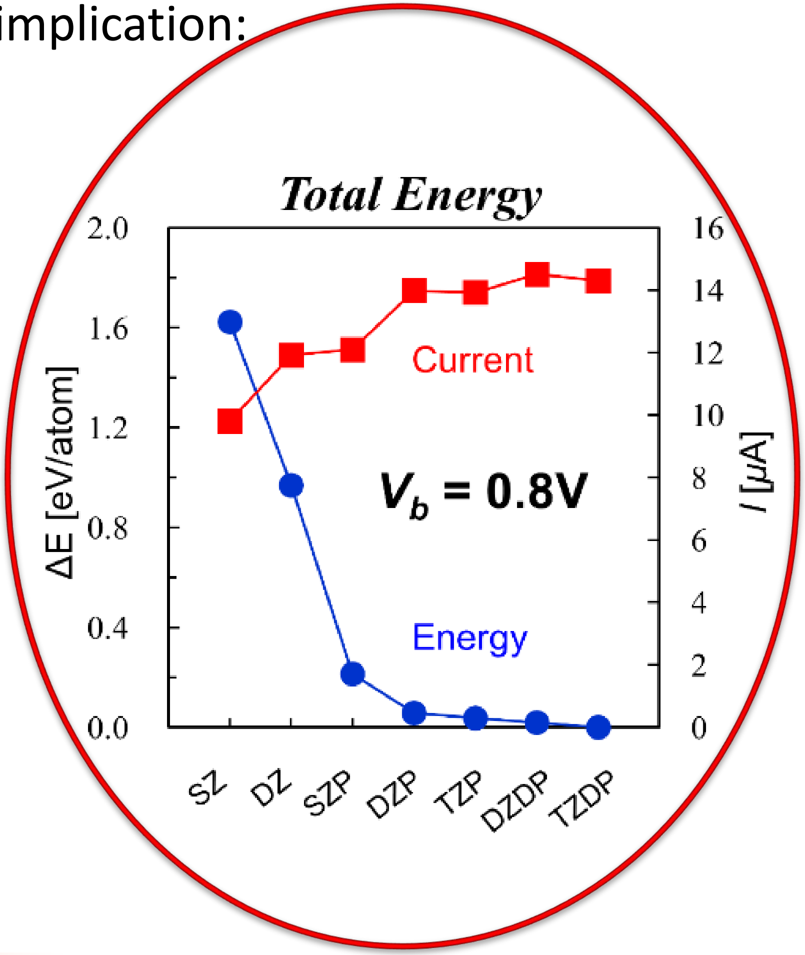
MS-DFT advantage 1. "Non-equilibrium" total energy

- MS-DFT (microcanonical) vs NEGF (grand-canonical) → Key implication:









Dr. Han Seul Kim

Dr. Juho Lee

J. Lee, H. Kim, & YHK,
Adv. Sci. **7**, 2001038
(2020)

2. Quasi-Fermi levels (Electrochemical potential drop)

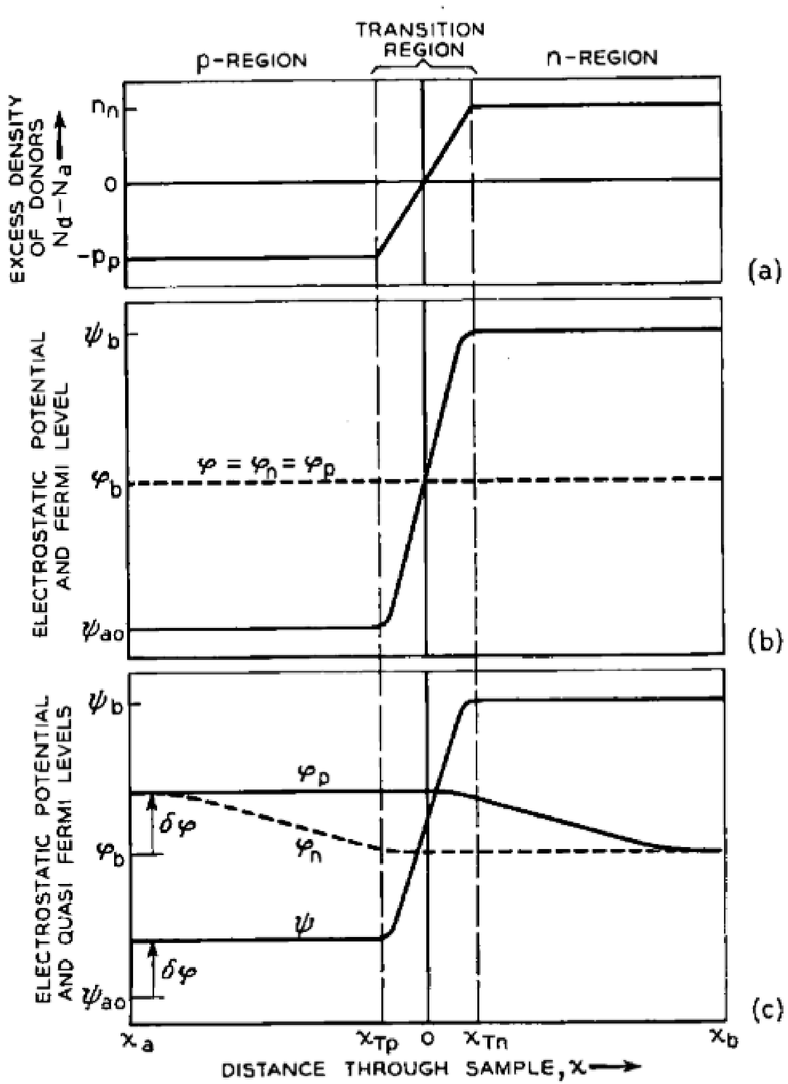
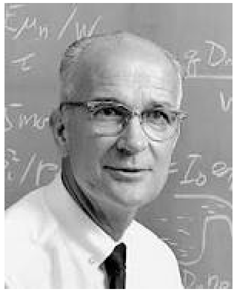


Fig. 6—Simplified model of a p-n junction.



William Shockley
(1910~1989)

Nobel Prize in Physics 1956

- ***p-n junction***

  Shockley, Bell Sys. Tech. J. **28**, 435 (1949)
- ***e-h recombination***

  Shockley-Read, Phys. Rev. **87**, 835 (1952)
- ***Solar cell***

  Shockley-Queisser, J. Appl. Phys. **32**, 510 (1961)

N.B.

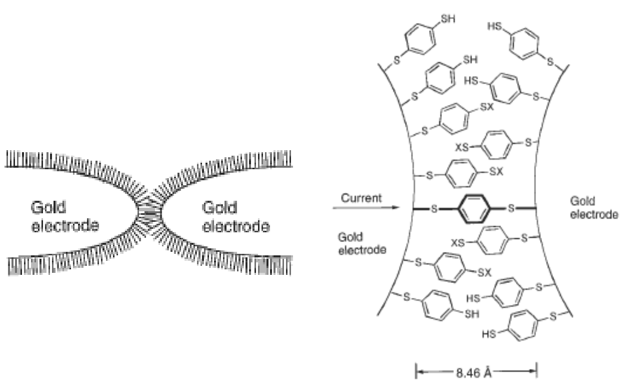
After 70 years since its inception,

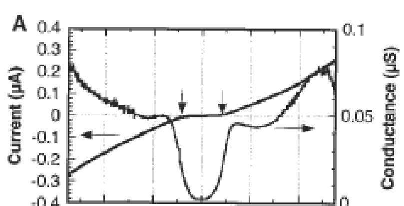
NO 1st-principles calculations of QFLs

Explicit (implicit) QFLs within MS-DFT (DFT-NEGF)

e.g. Molecular electronic devices

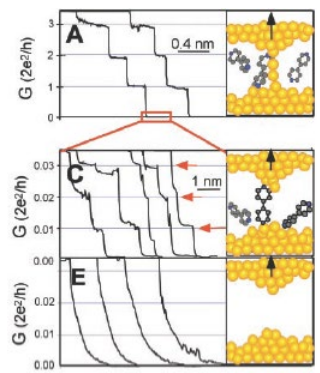
Mark Reed
(1955~2021)

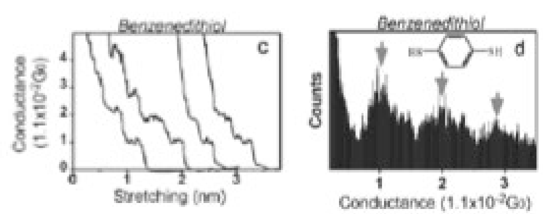




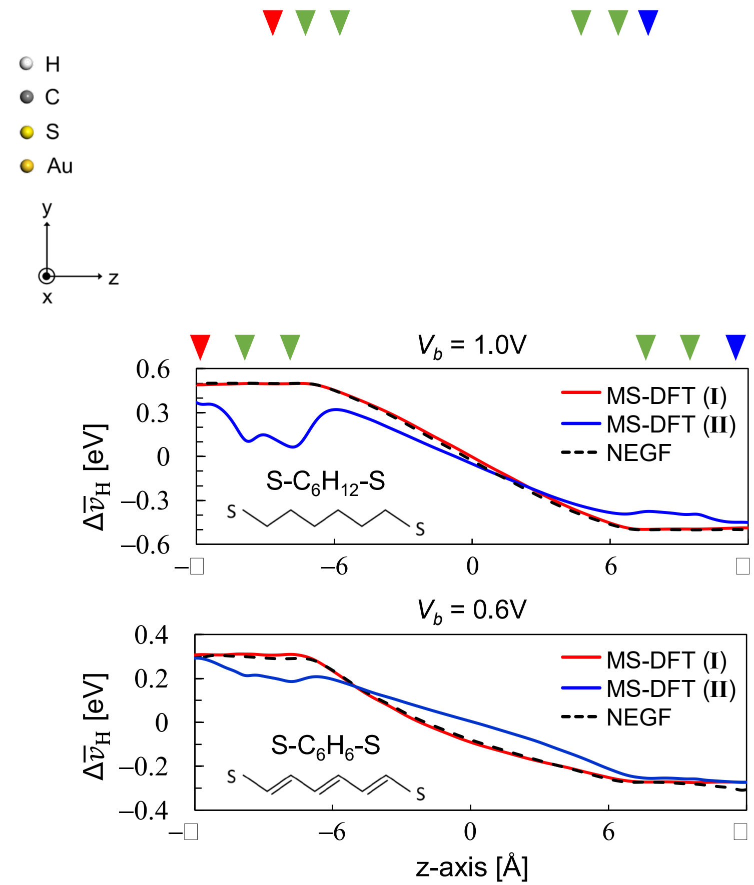
Science (1997)

Nongjian Tao
(1963~2020)





Science (2003)

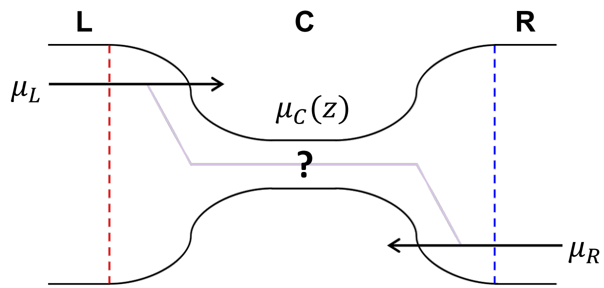


Hexane-dithiolate

Hexatriene-dithiolate

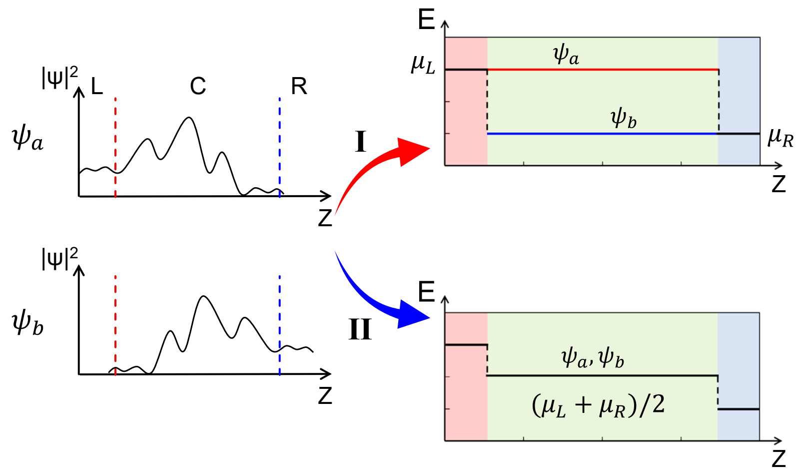
Explicit (implicit) QFLs within MS-DFT (DFT-NEGF)

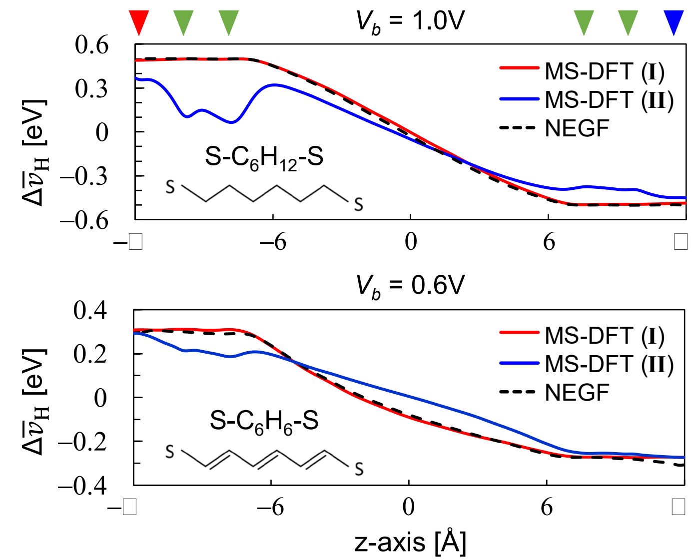
- Occupation rule? → Important to maintain the separate (non-local) QFLs!



Juho Lee

Hyun Woo Yeo





Hexane-dithiolate

Hexatriene-dithiolate

J. Lee, H. Yeo, & YHK, PNAS **117**, 10142 (2020)

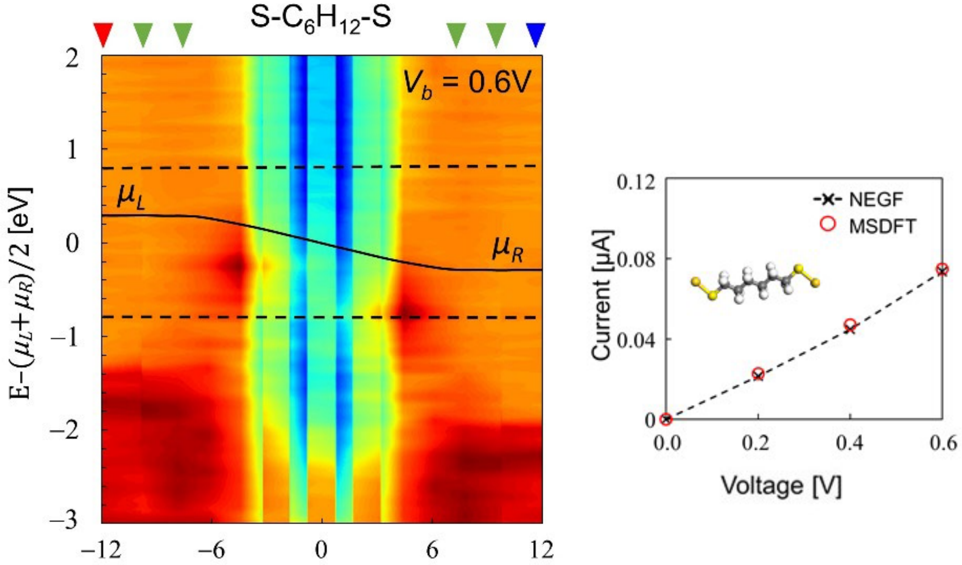
cf.
$$n(\vec{r}) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} dE\,\mathbf{G}^{\mathrm{n}}(\vec{r},E)$$
$$\approx \frac{1}{2\pi}\int_{-\infty}^{+\infty} dE\,[f_1\mathbf{A}_1 + f_2\mathbf{A}_2]$$
$\mathbf{A}_1 = \mathbf{G\Gamma_1 G^+}$, $\mathbf{A}_2 = \mathbf{G\Gamma_2 G^+}$

$$\psi_i(\vec{r}) \in \begin{cases} \psi_i^{\mathrm{L}} \text{ if } \int_{\mathrm{L}} |\psi_i(\vec{r})|^2 d^3r > \int_{\mathrm{C/R}} |\psi_i(\vec{r})|^2 d^3r, \\ \psi_i^{\mathrm{C}} \text{ if } \int_{\mathrm{C}} |\psi_i(\vec{r})|^2 d^3r > \int_{\mathrm{L/R}} |\psi_i(\vec{r})|^2 d^3r, \\ \psi_i^{\mathrm{R}} \text{ if } \int_{\mathrm{R}} |\psi_i(\vec{r})|^2 d^3r > \int_{\mathrm{L/C}} |\psi_i(\vec{r})|^2 d^3r \end{cases}$$

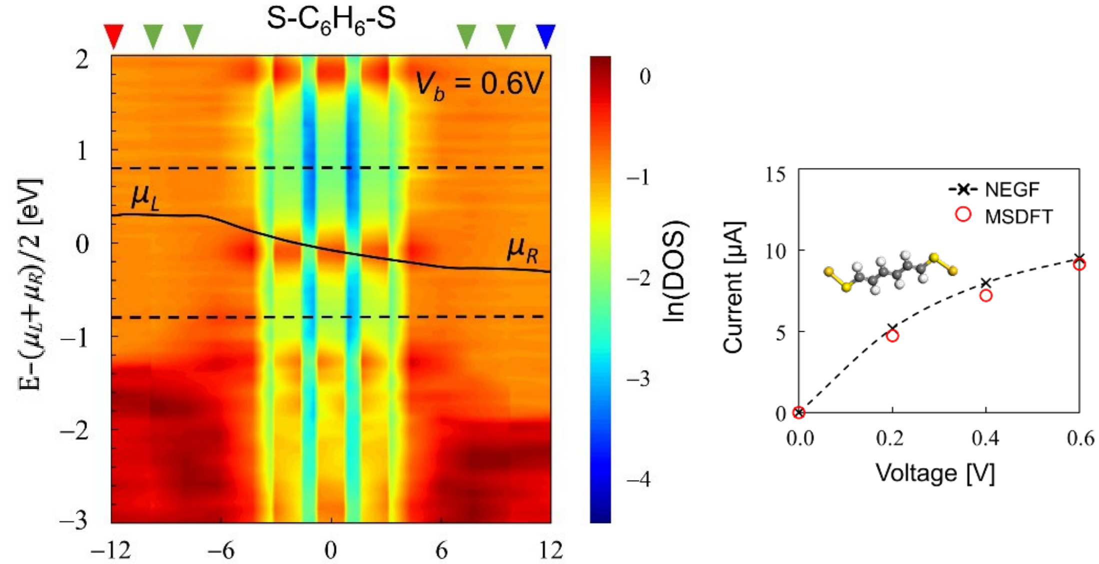
QFL splitting: Where is the "voltage" drop?

- Electrostatic potential drop: Why nonlinear drop @ hexatriene-dithiolate?

Hexane-dithiolate (insulator)



Hexatriene-dithiolate (semiconductor)



Electrochemical potential drop

$$V = \frac{\mu_1(\mathbf{r}_2) - \mu_1(\mathbf{r}_2)}{e} = \phi(\mathbf{r}_2) - \phi(\mathbf{r}_1) + \frac{\bar{\mu}(\mathbf{r}_2) - \bar{\mu}(\mathbf{r}_1)}{e}$$

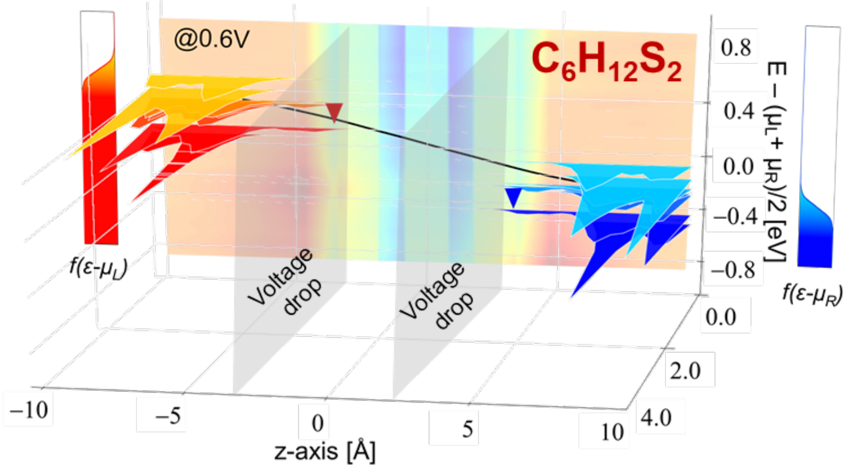
Electrostatic potential drop

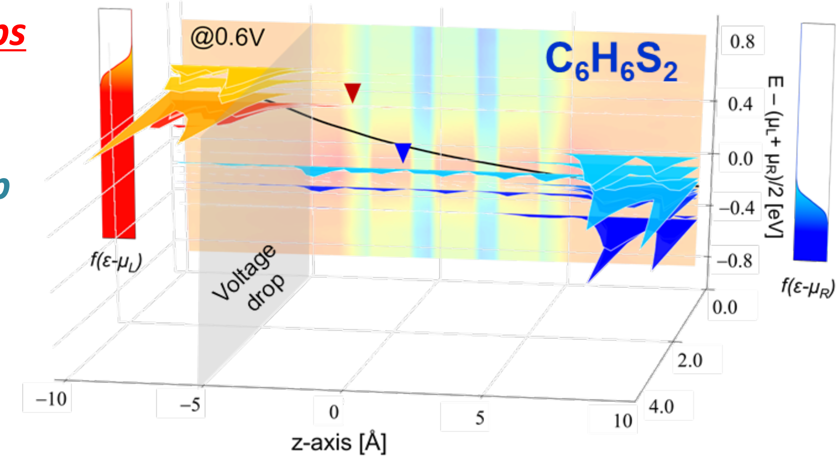
Chemical potential drop

Electrostatic potential drops

Hexane-dithiolate

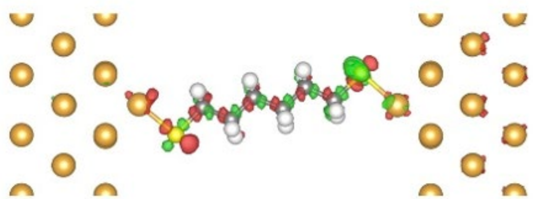
Hexatriene-dithiolate

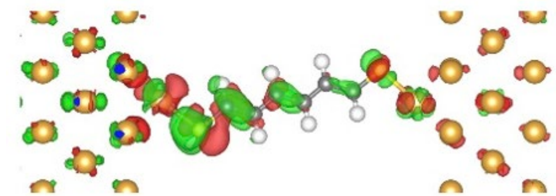




"Voltage" drops

Electrostatic potential drop

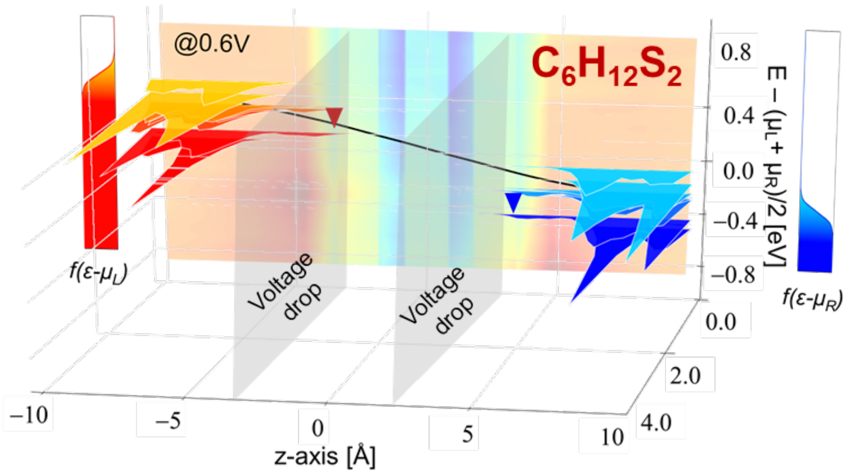




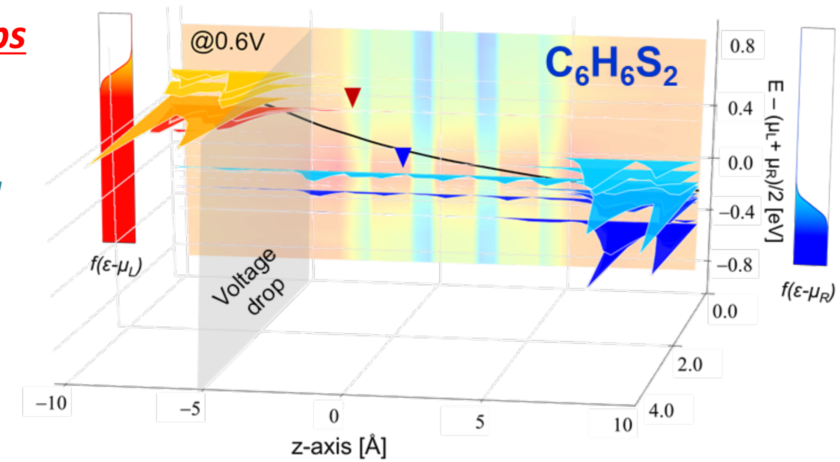
Landauer residual resistivity dipole

Electrochemical potential drops (QFLs)

Hexane-dithiolate

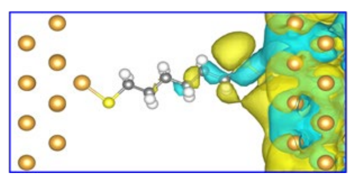


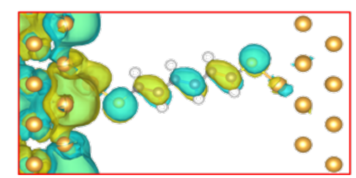
Hexatriene-dithiolate

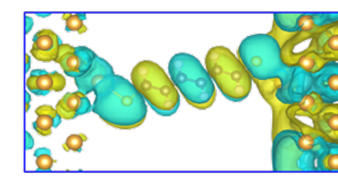


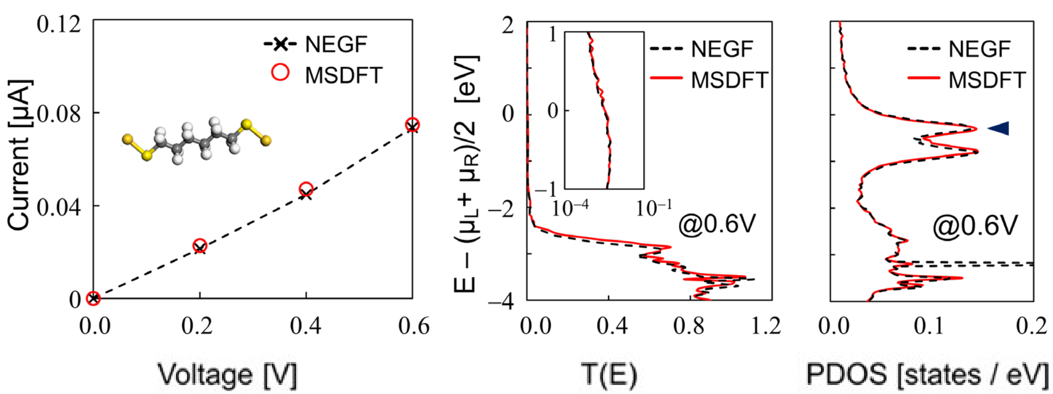
"Voltage" drops

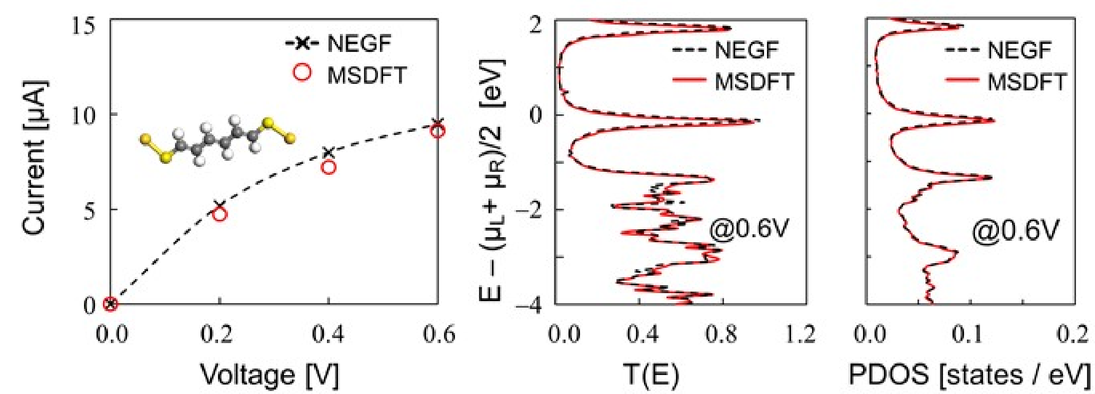
Quasi-Fermi level splitting







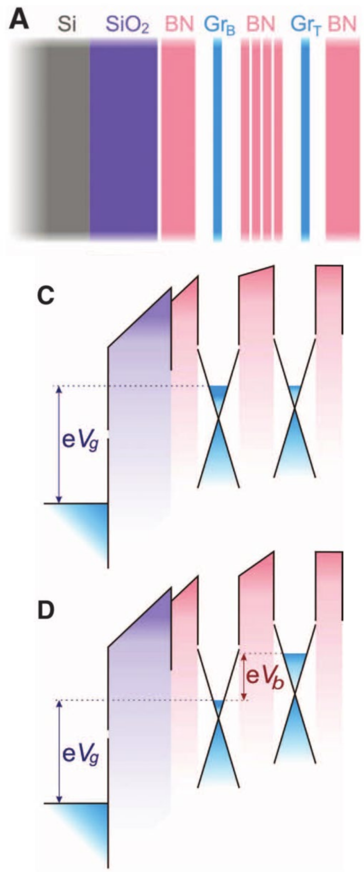




3. 2D vdW devices: e.g. Gr/hBN/Gr heterojunctions

Vertical tunneling field effect transistor (FET)

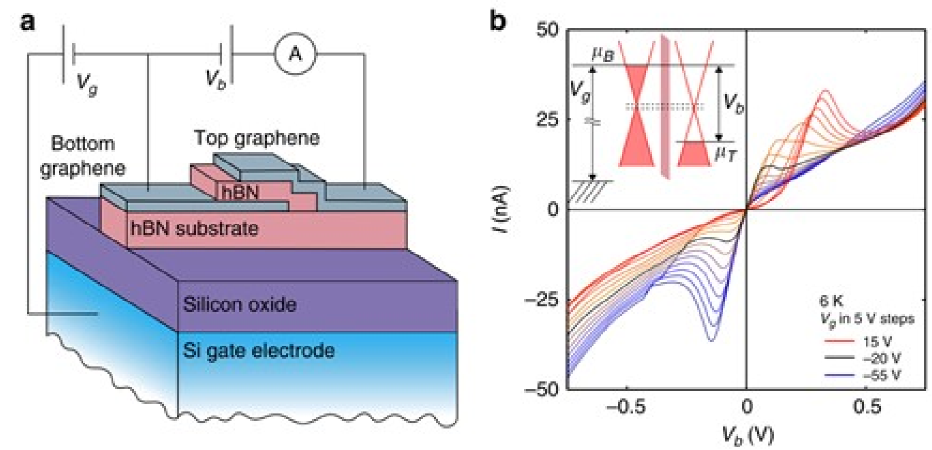
L. Britnell *et al. Science* **335,** 947 (2012)



Modulation of tunneling currents
→ On/Off ≈ 1×10^4

- *Negative Differential Resistance (NDR)*

L. Britnell *et al. Nat. Commun.* 4, 1794 (2013)



- *High photocurrent*

L. Britnell *et al. Science* 340, 1311 (2013), etc.

- *Chiral quantum states*

J. Wallbank *et al. Science* 353, 6299 (2016), etc.

- *Giant tunneling magnetoresistance*

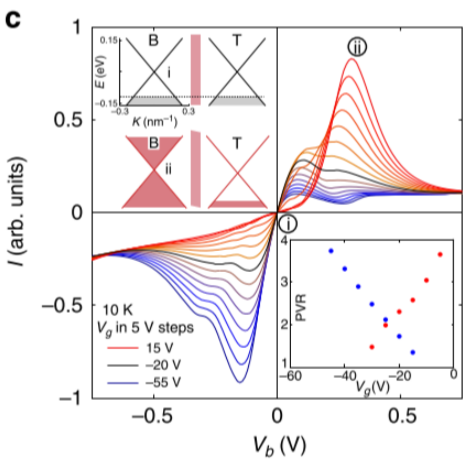
T. Song *et al. Science* 360, 1214 (2018), etc.

- *etc.*

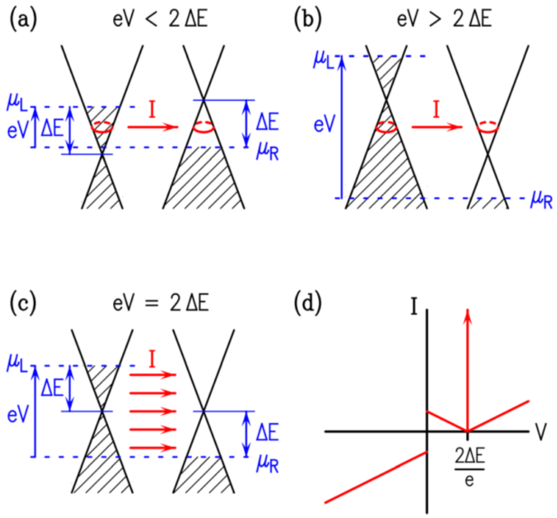
Only semi-classical theory (not NEGF)

- Semi-classical Bardeen approach

$$I = g_V \frac{4\pi e}{\hbar} \sum_{\alpha,\beta} |M_{\alpha\beta}|^2 [f_L(E_\alpha) - f_R(E_\beta)] \delta(E_\alpha - E_\beta)$$

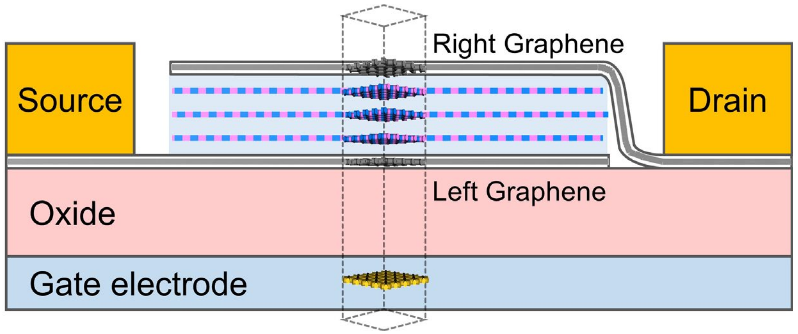


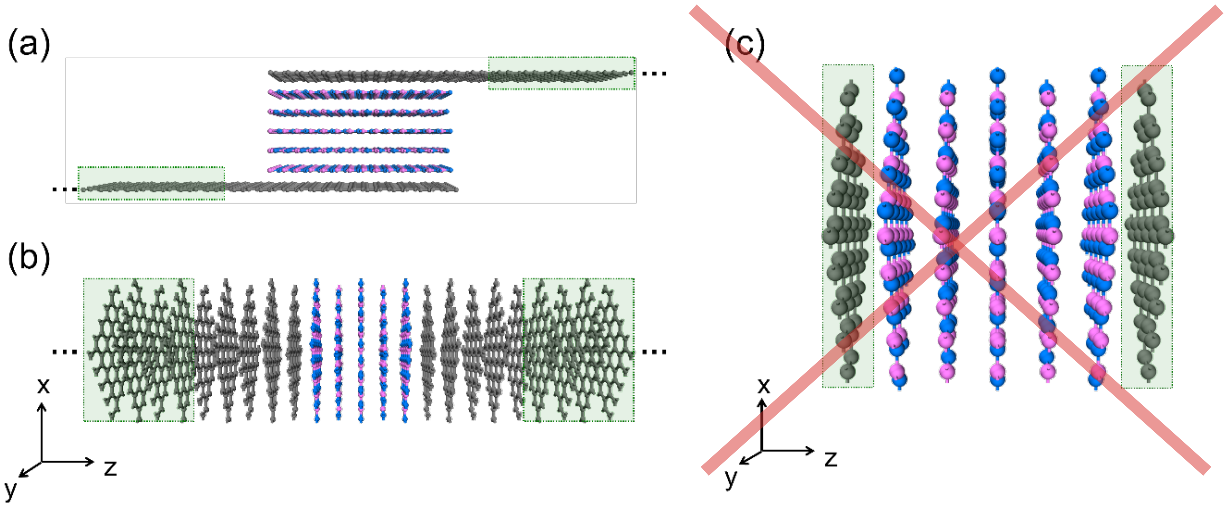
L. Britnell *et al.*
Nat. Commun. **4,** 1794 (2013)



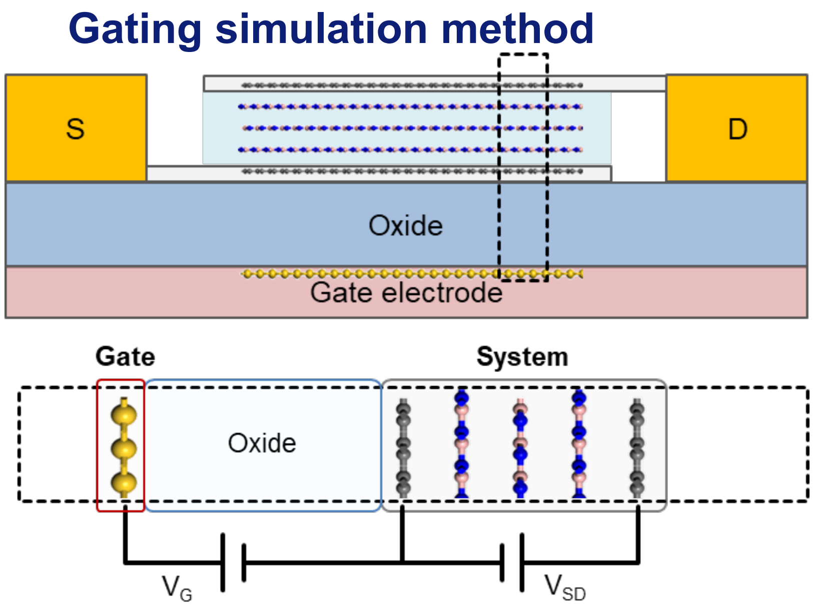
Feenstra *et al.*
J. Appl. Phys. **111,** 4 (2012)

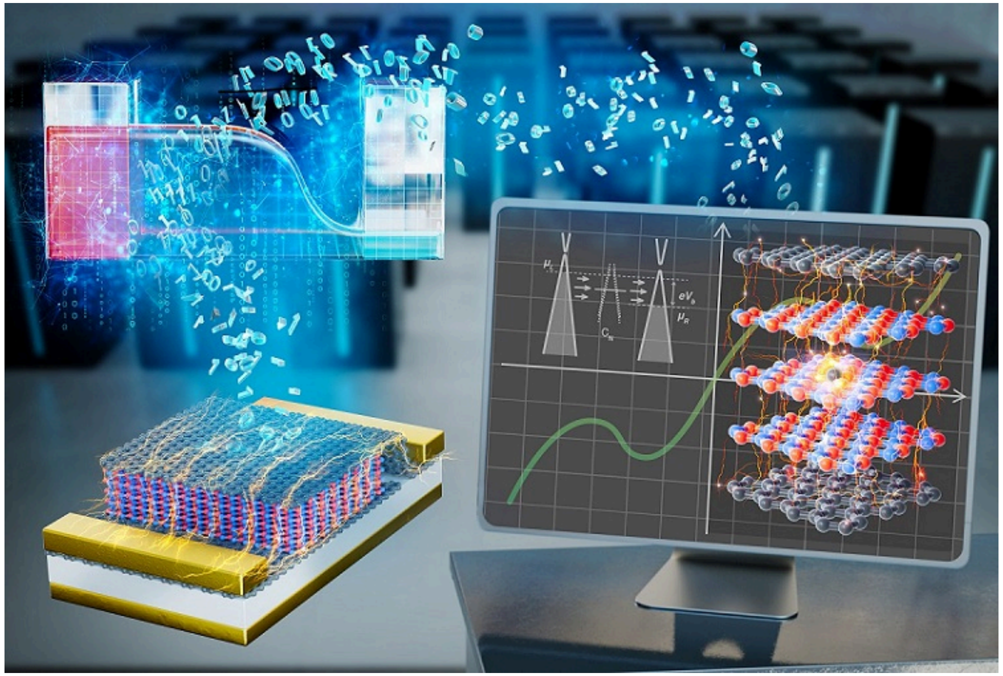
- Difficulty with DFT-NEGF





MS-DFT for graphene tunneling "FET"





1. "Constrained search":

   V_G as a constraint that precedes V_{SD}

2. Transmission:

$$T(E; V_b, V_g) = Tr\left[\boldsymbol{a}_L \, \mathbf{M} \, \boldsymbol{a}_R \, \mathbf{M}^{\dagger}\right]$$

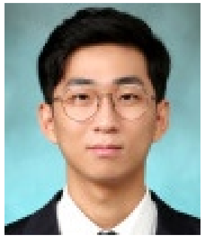
T.H. Kim, J. Lee, R.-G. Lee, & YHK, Npj Comput. Mater. **8**, 50 (2022)

Son *et al.*, Appl. Surf. Sci. **581**, 152396 (2022)

Seo *et al.*, Adv. Mater. **33**, 2102980 (2021)

Taehyung Kim

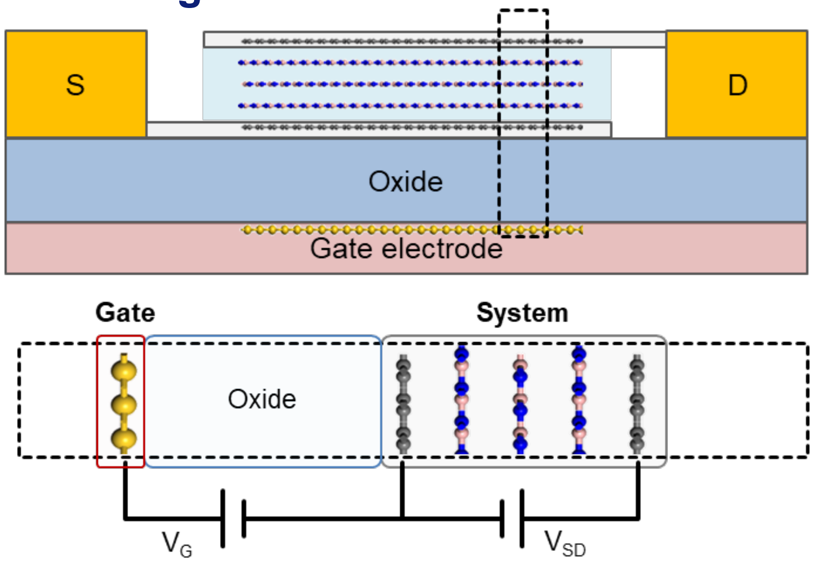
Juho Lee



Ryong Gyu Lee

MS-DFT for graphene TFET: $V_G = +1V$

Gating simulation method



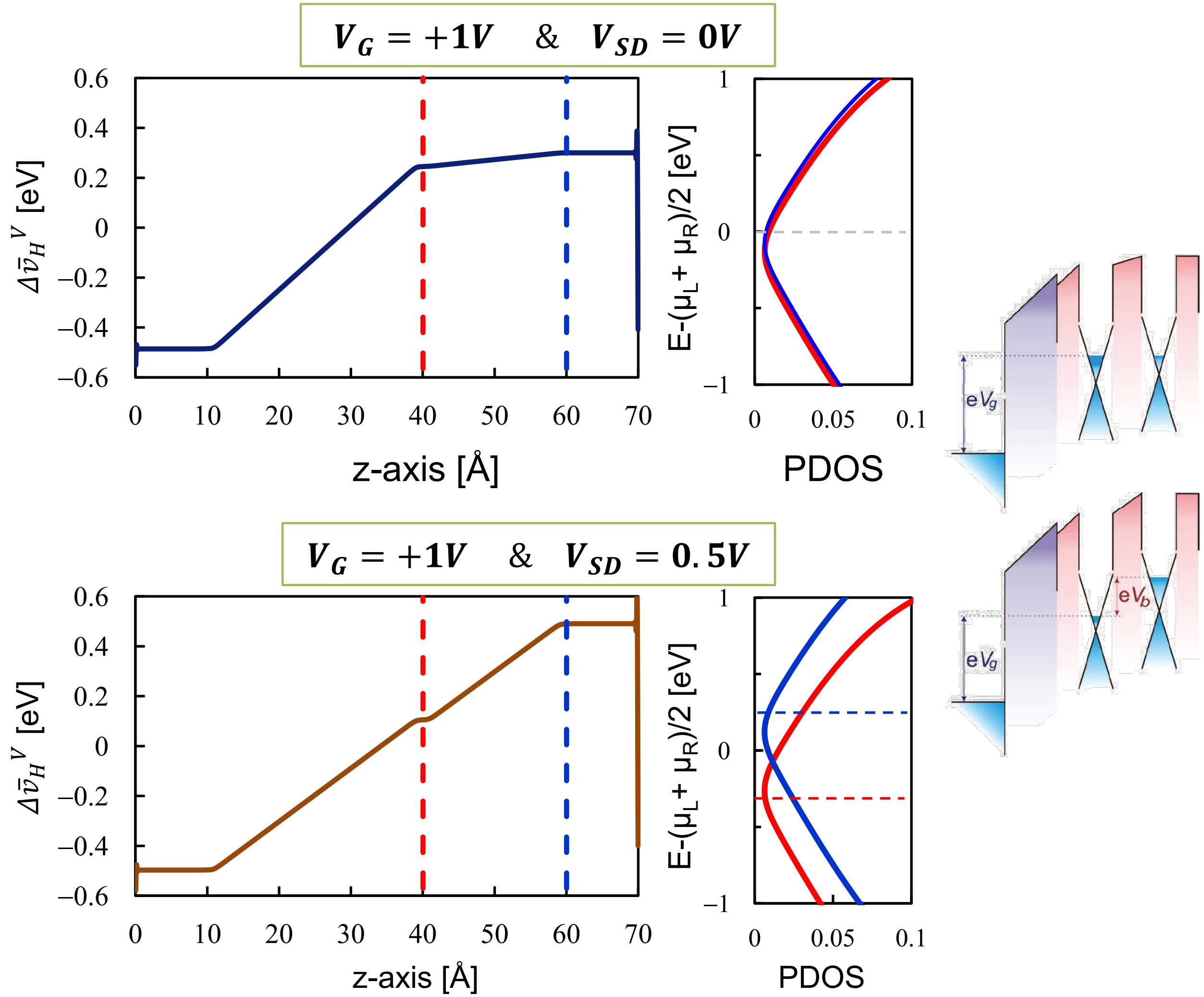
1. "Constrained search":

   V_G as a constraint that precedes V_{SD}

2. Transmission:

$$T\left(E; V_b, V_g\right) = Tr\left[\boldsymbol{a}_L\, \mathbf{M}\, \boldsymbol{a}_R\, \mathbf{M}^{\dagger}\right]$$

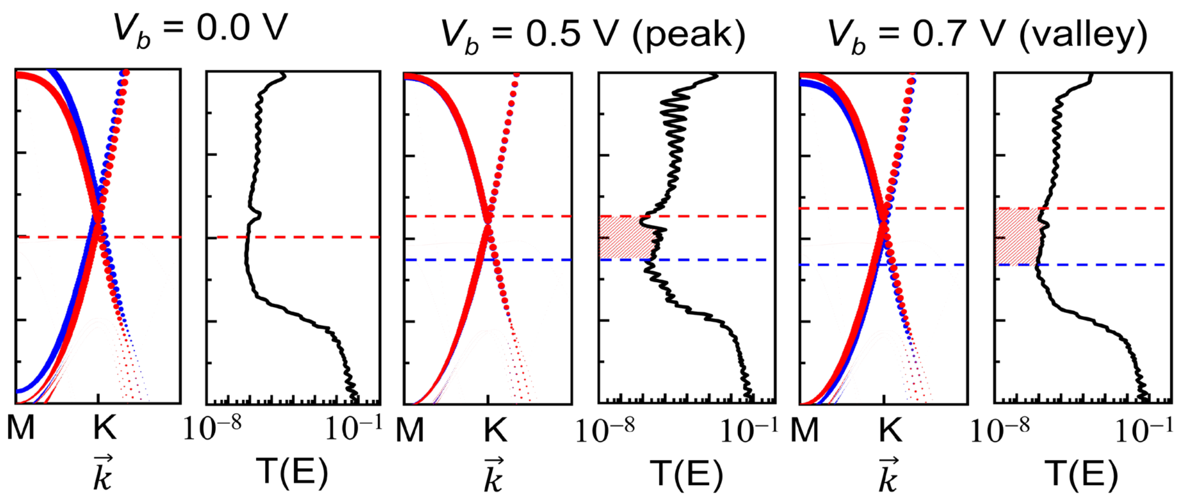
$$\Delta\bar{v}_H^V(\vec{r}; V_{SD}, V_G) = \bar{v}^V(\vec{r}; V_{SD}, V_G) - \bar{v}^0(\vec{r}; 0, 0)$$

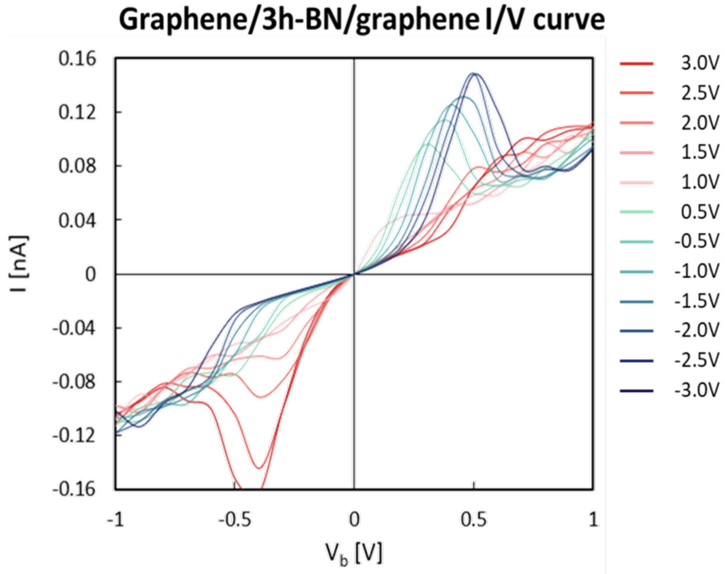


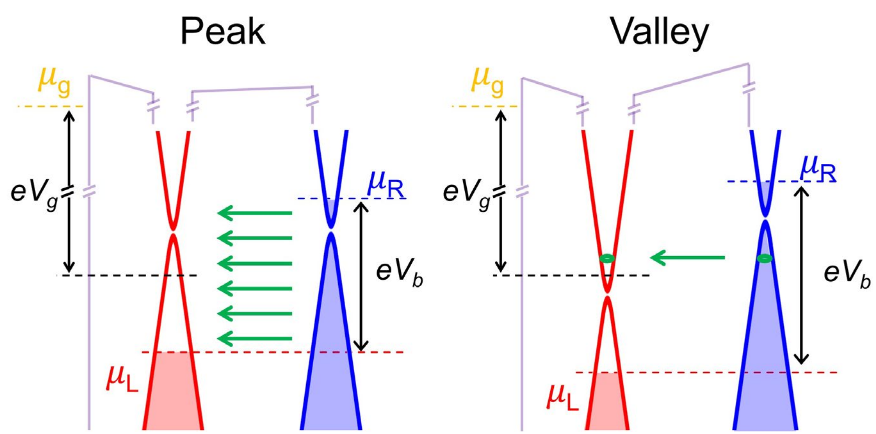
- Quantum capacitance → Field partial penetration

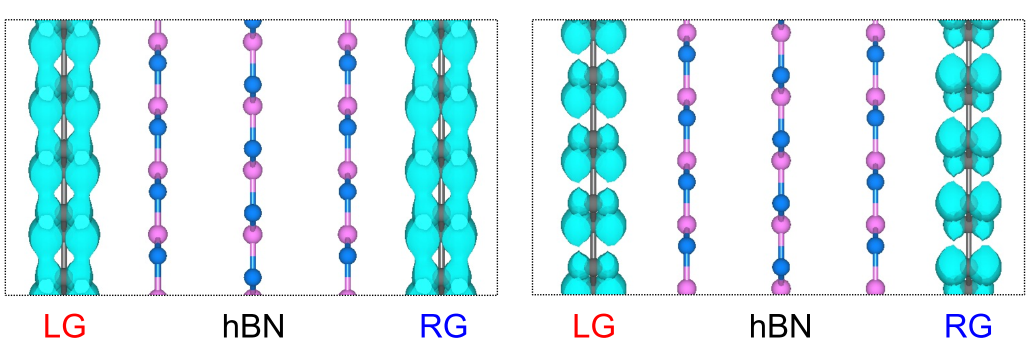
NDR @ Gr/pristine hBN/Gr TFET ← MS-DFT

$V_G = -2.5V$



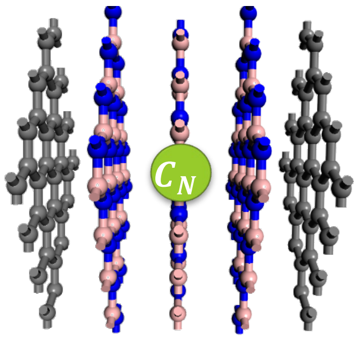


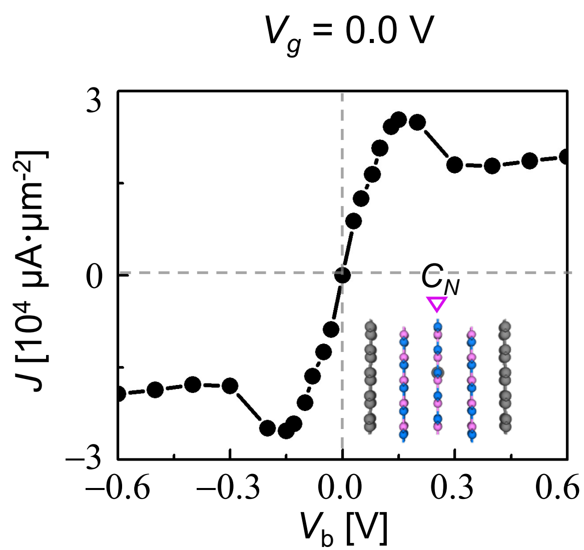




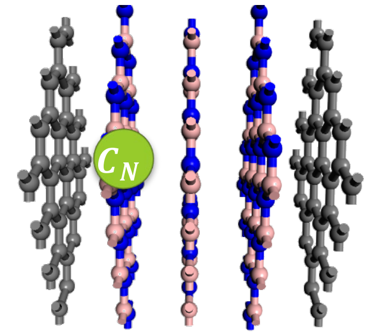
Gr/defective hBN/Gr: I-V & voltage drop

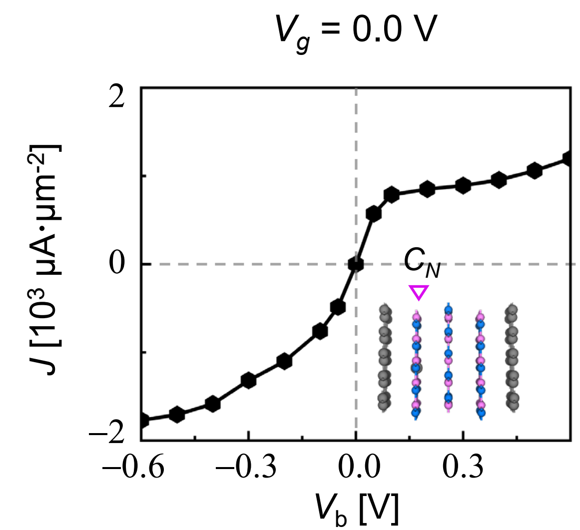
C_N defect @ middle hBN



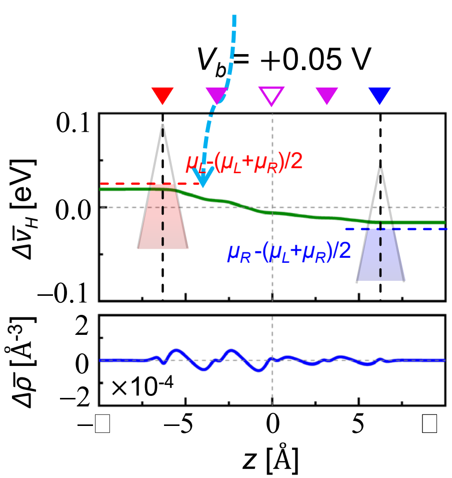


C_N defect @ interfacial hBN

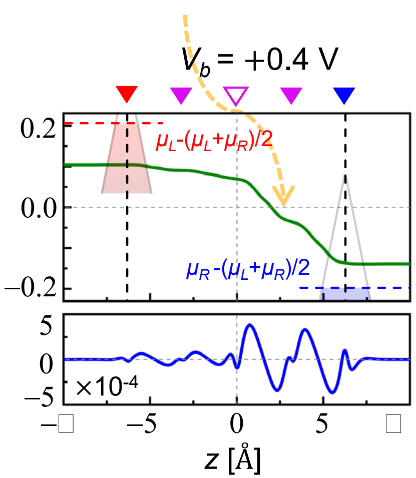




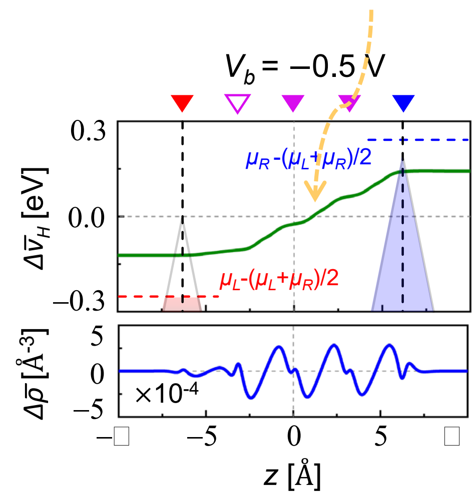
V drop @ left



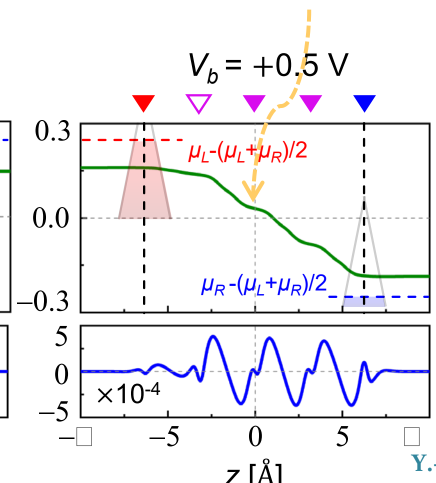
V drop @ right



V drop @ right

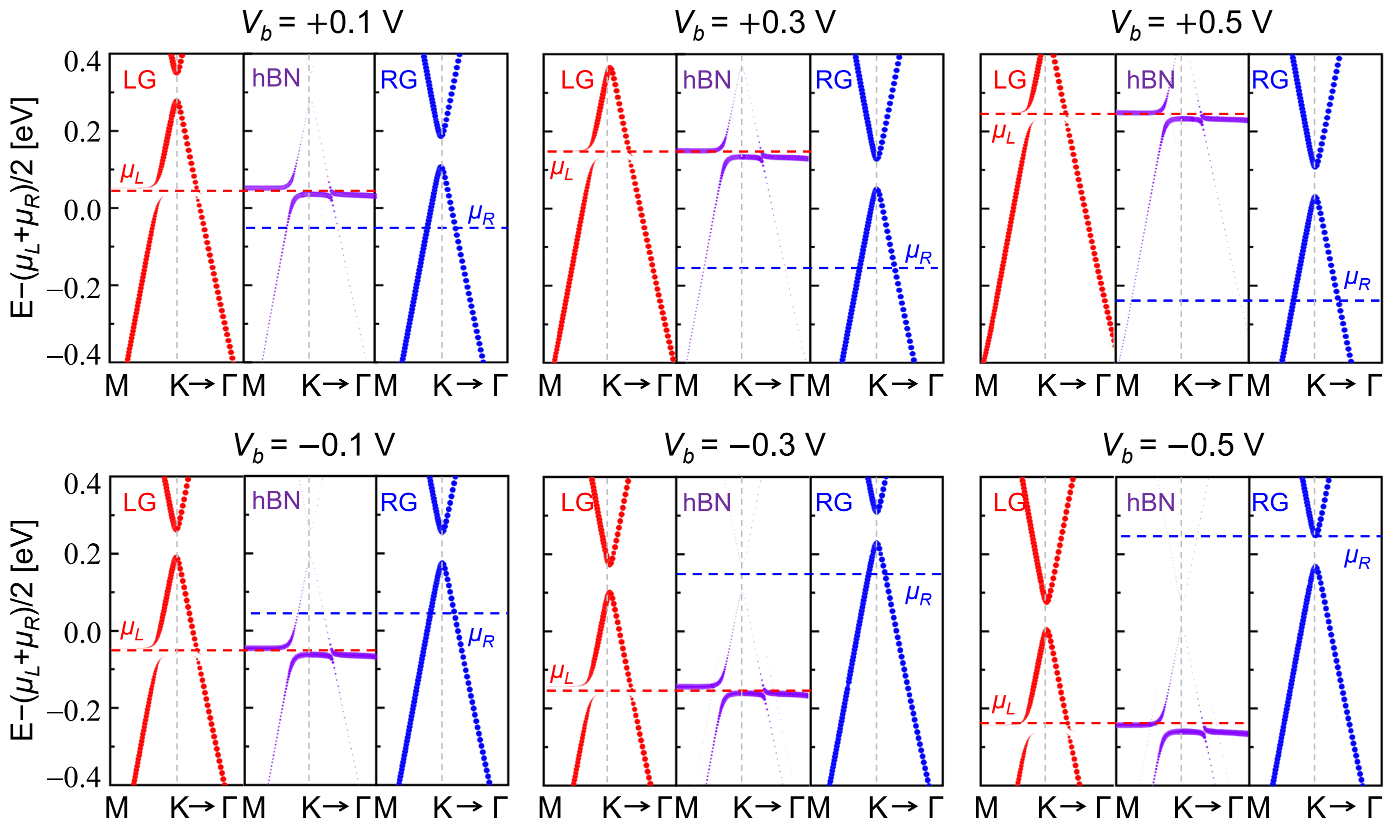


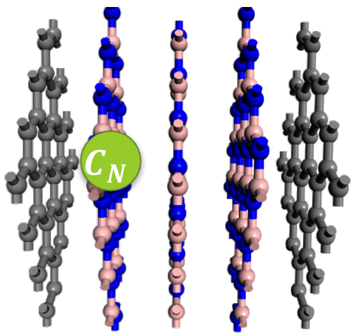
V drop @ right

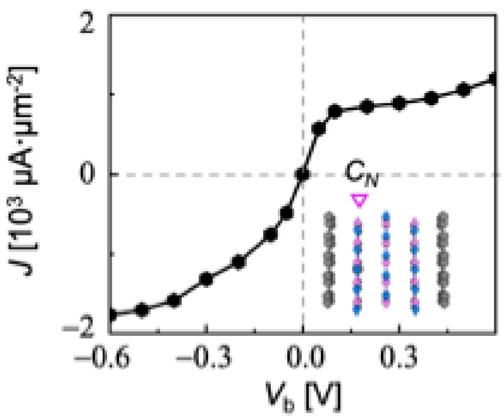


Gr/defective hBN/Gr: C_N @ interfacial hBN → No NDR

T.H. Kim, J. Lee, R.-G. Lee, & YHK,
Npj Comput. Mater. **8**, 50 (2022)



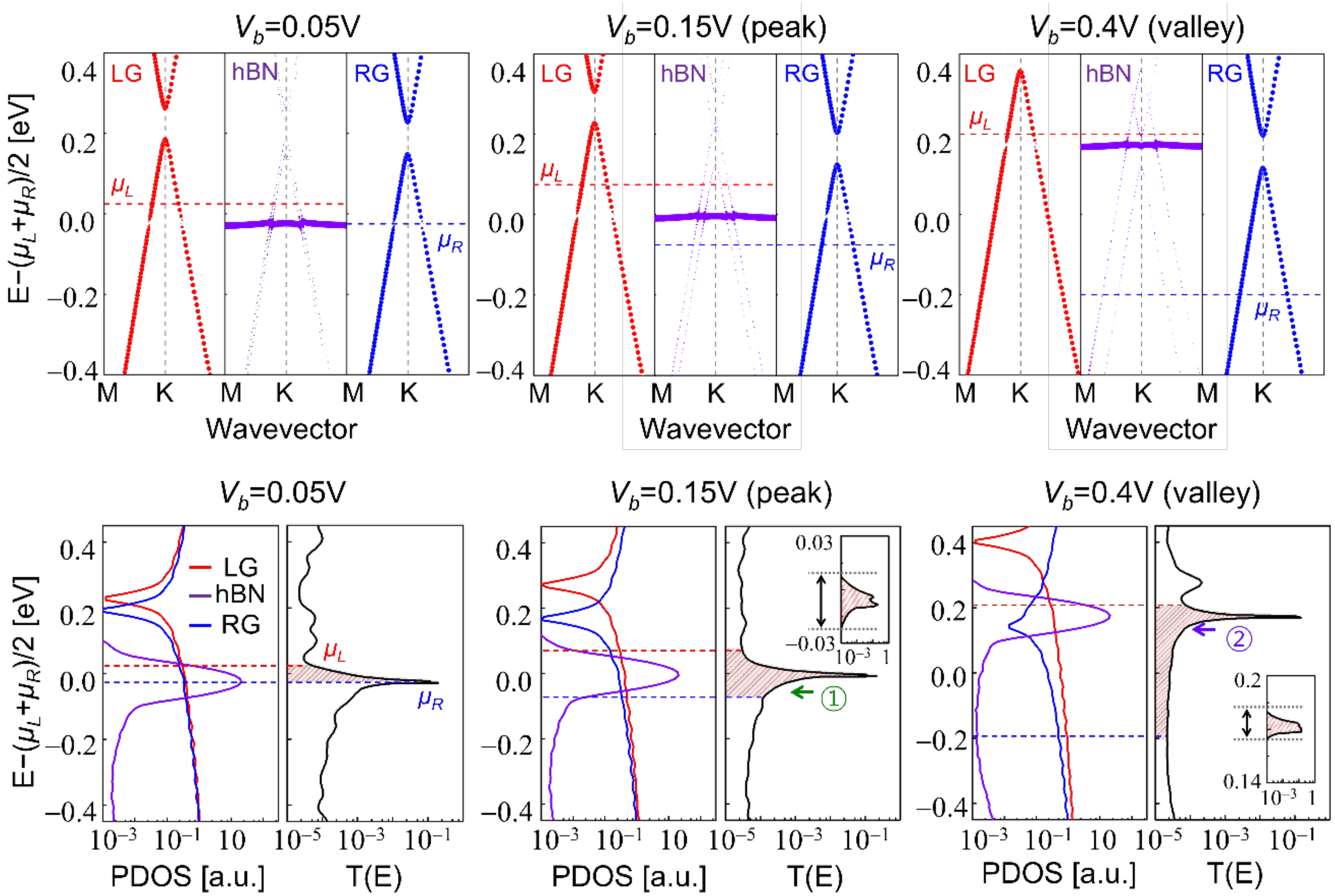


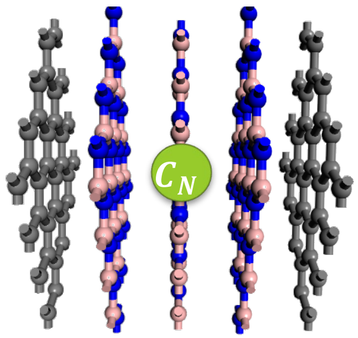


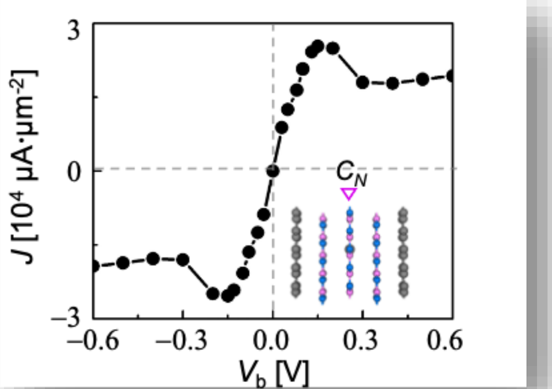
- Pinning of C_N defect @ left Gr

Gr/defective hBN/Gr: C_N @ middle hBN → symmetric NDR

T.H. Kim, J. Lee, R.-G. Lee, & YHK, Npj Comput. Mater. **8**, 50 (2022)





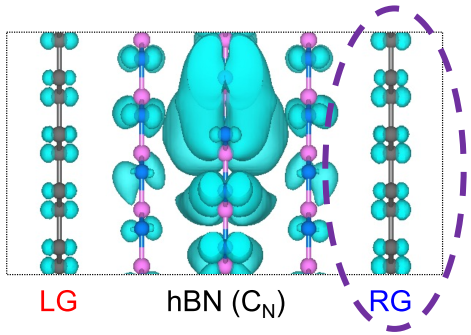


- Self-consistent filling of C_N defect levels → upshift with V_b
- C_N defect level-mediated symmetric NDR

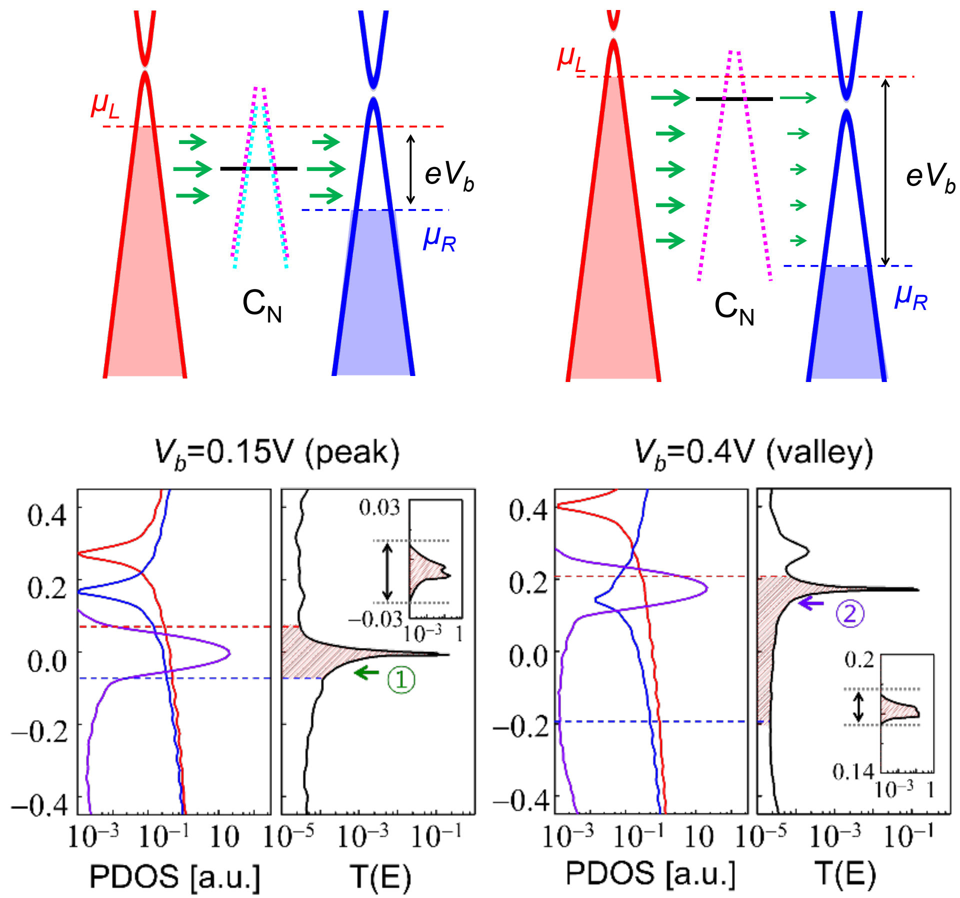
Gr/defective hBN/Gr: C_N @ middle hBN → QH-NDR

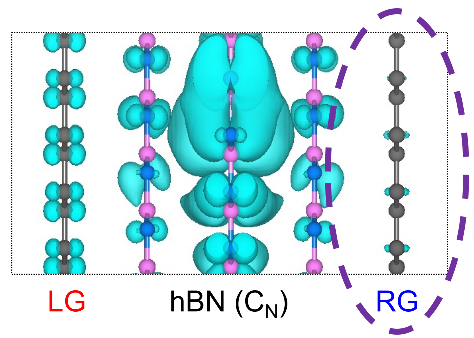
Quantum-Hybridization NDR

T.H. Kim, J. Lee, R.-G. Lee, & YHK, Npj Comput. Mater. **8**, 50 (2022)



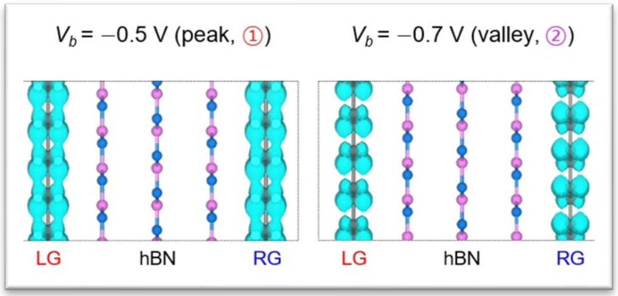
Quantum hybridization (QH): Strong

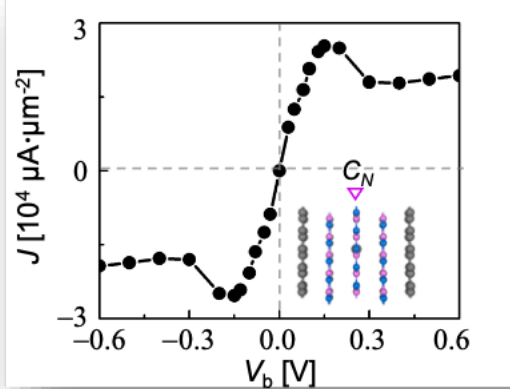




Quantum hybridization (QH): Weak

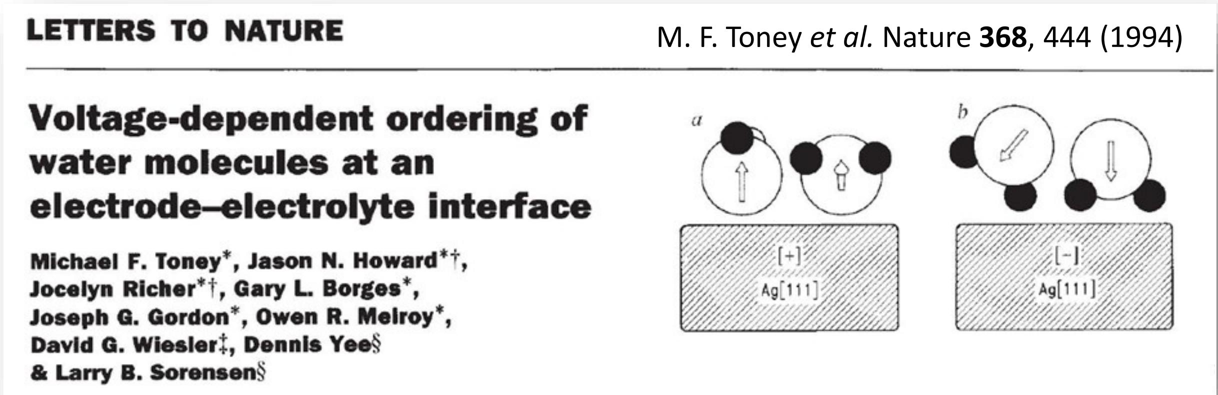
cf.





- Self-consistent filling of C_N defect levels → upshift with V_b
- C_N defect level-mediated NDR → QH-NDR

4. Interfacial water from first-principles?

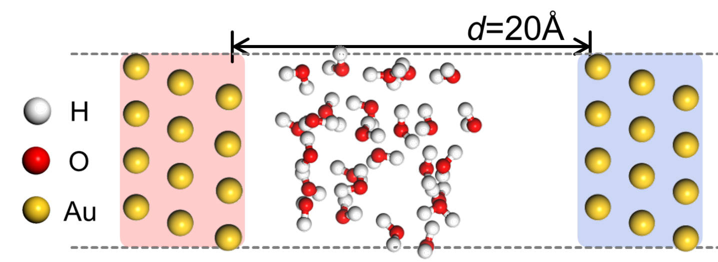


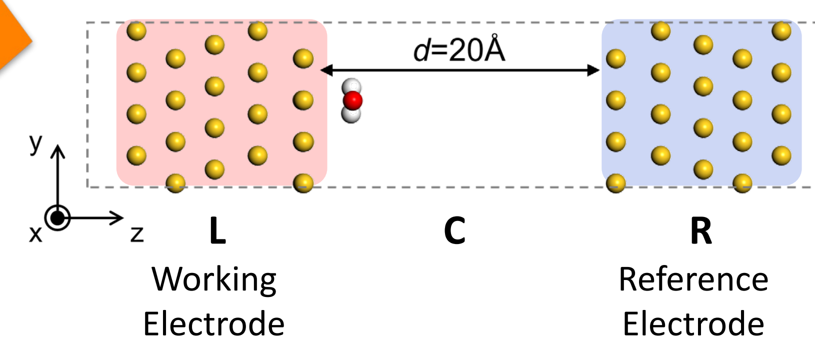
LETTERS TO NATURE — M. F. Toney *et al.* Nature **368**, 444 (1994)

Voltage-dependent ordering of water molecules at an electrode–electrolyte interface

Michael F. Toney*, Jason N. Howard*†, Jocelyn Richer*†, Gary L. Borges*, Joseph G. Gordon*, Owen R. Melroy*, David G. Wiesler‡, Dennis Yee§ & Larry B. Sorensen§

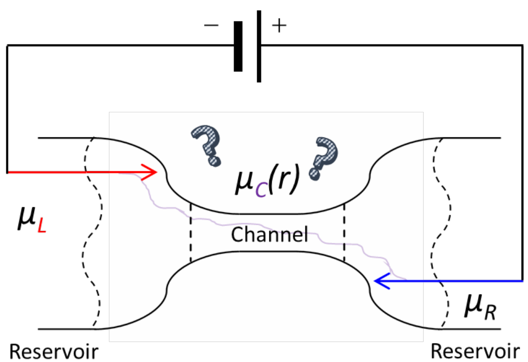
Models

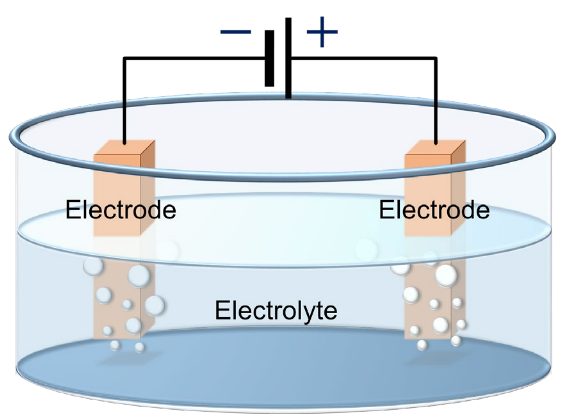




Quantum transport → Electrolytic cell

$V = \Delta\mu = \mu_L - \mu_R$





$$\Phi = -\frac{V_b}{2} = -\frac{(\mu_L - \mu_R)}{2e}$$

cf. Interfacial water ← NEGF

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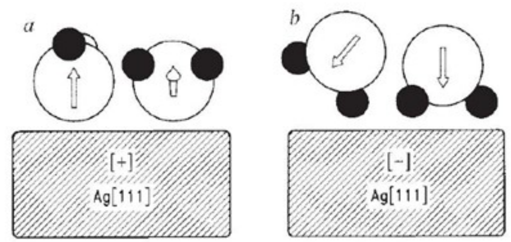
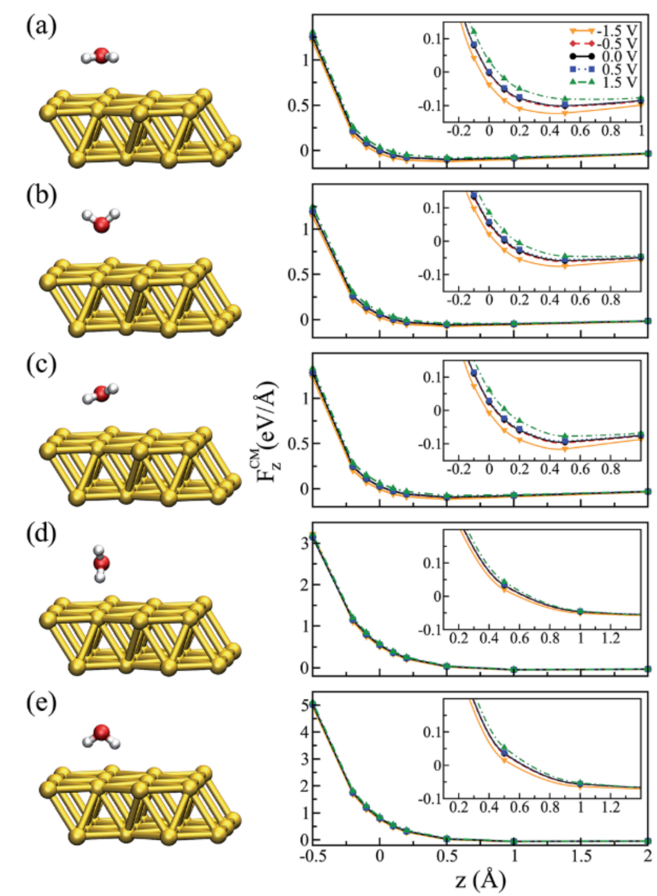


?

Chem. Sci. **9**, 62 (2018)

Bias-dependent local structure of water molecules at a metallic interface†

Luana S. Pedroza,[*ab] Pedro Brandimarte,[cd] Alexandre Reily Rocha[e] and M.-V. Fernández-Serra[fg]

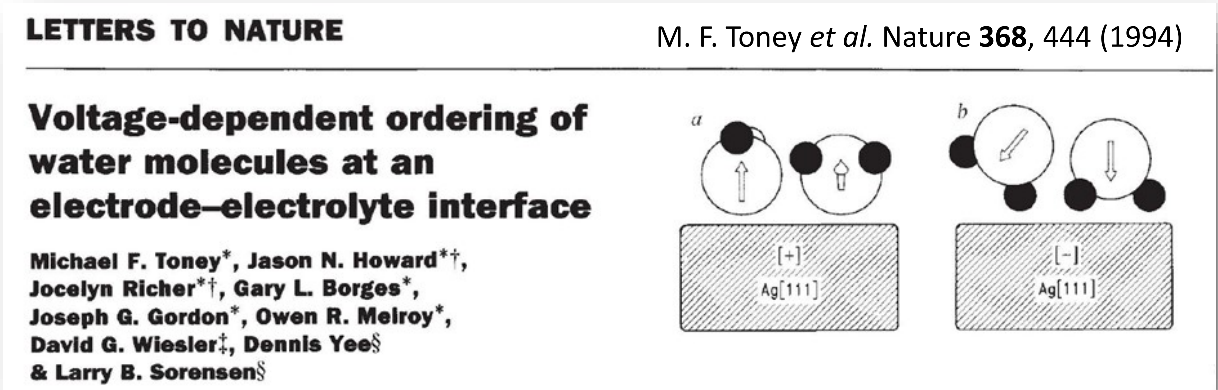


- Hellmann-Feynman forces:

$$\vec{F}_I = -\frac{\partial\langle\psi^{L/C/R}|\,\hat{H}|\psi^{L/C/R}\rangle}{\partial\vec{R}_I}$$

- But no energy … $\langle\psi^{L/C/R}|\,\hat{H}|\psi^{L/C/R}\rangle$?

Q. Interfacial water ← MS-DFT?



LETTERS TO NATURE

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?

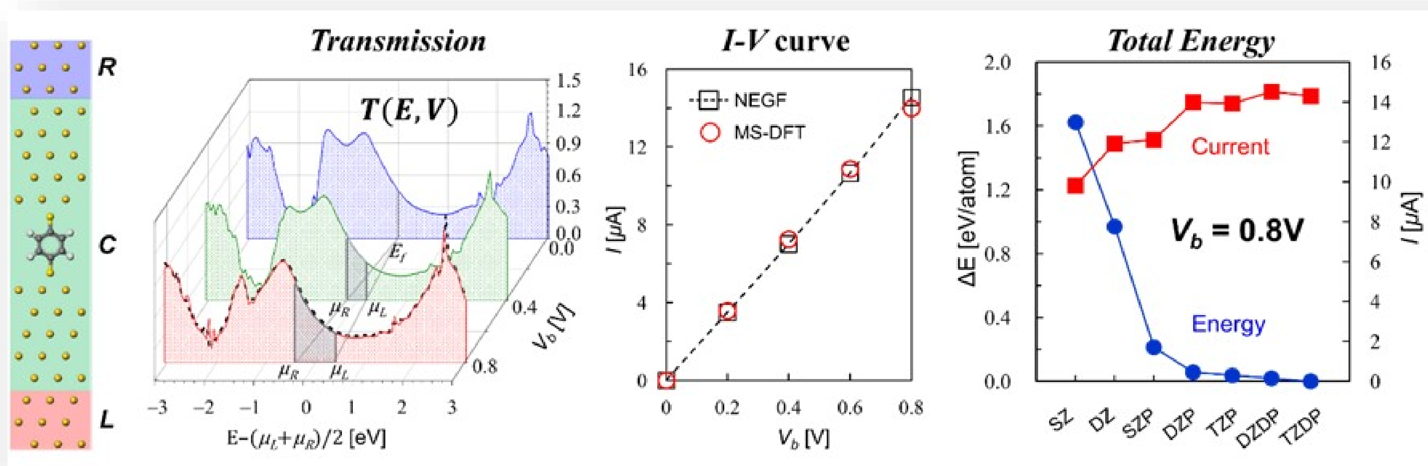
MS-DFT

Total energy E^V_{L+C+R}:

NOT enough!

→ Q. Appropriate

Free energy ?



Outline

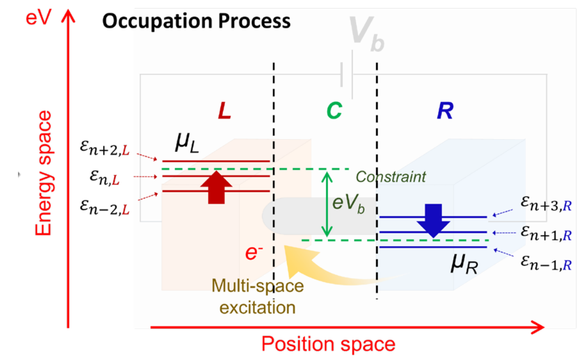
I. Background information: DFT, NEGF, & Landauer

II. MS-DFT: development & its applications

III. Summary

Summary

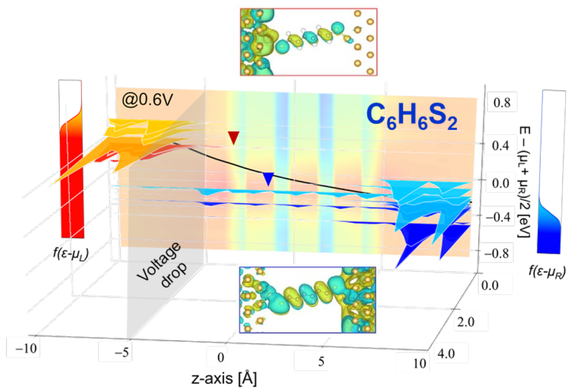
- "Multi-space excitation" for quantum transport
  - An alternative to the Landauer viewpoint
  - Formulation of MS-DFT (vs. NEGF)

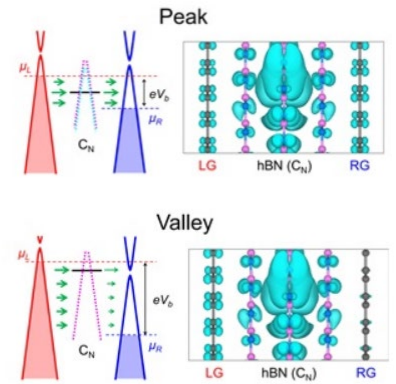


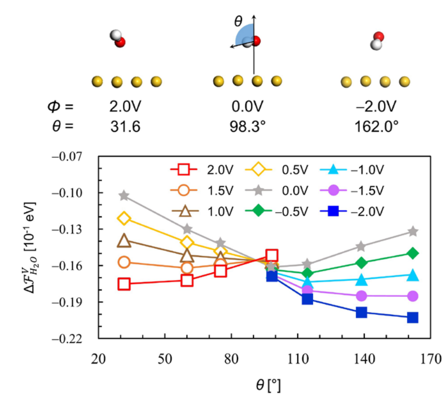
- Advantages and Applications
  - Quasi-Fermi levels: "Voltage drop"
  - Graphene-based nanodevices
  - Total energy

  → Electric enthalpy (of formation)

  → Interfacial water (and beyond …)







Acknowledgements

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http://nanocore.kaist.ac.kr/yhklab

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Funding

HYBRID INTERFACE MATERIALS

NRF 한국연구재단 National Research Foundation of Korea

KAIST

SAMSUNG ELECTRONICS

LG Display

감사합니다.

Thank you!