Device Simulation for Carbon Nanotube Electronics

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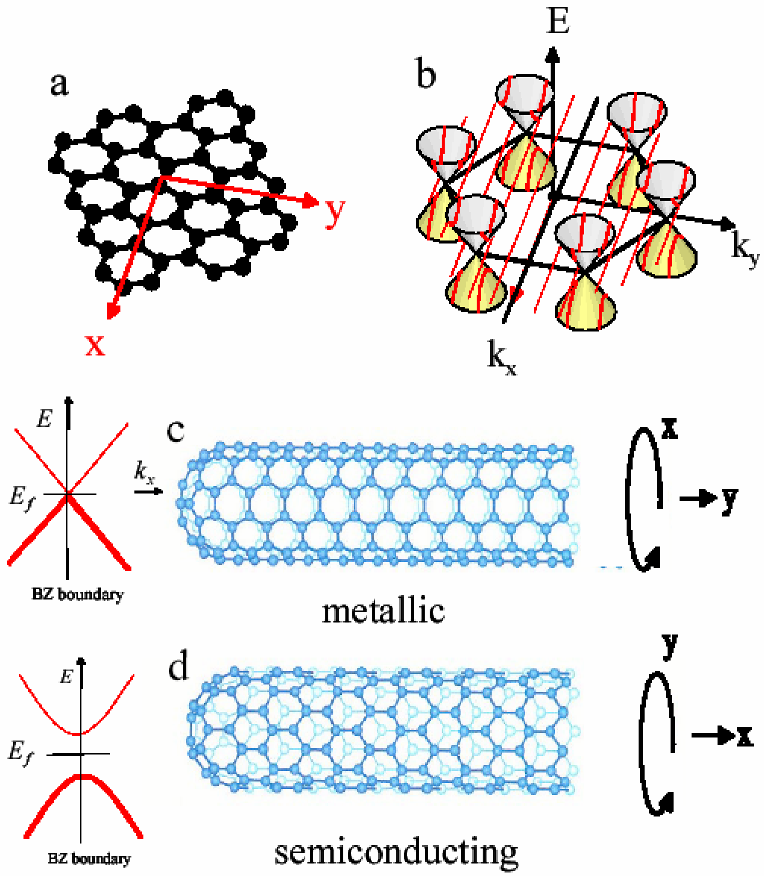
1. Introduction
2. NEGF formalism
3. Simulation Approach
4. Device Analysis
5. Summary

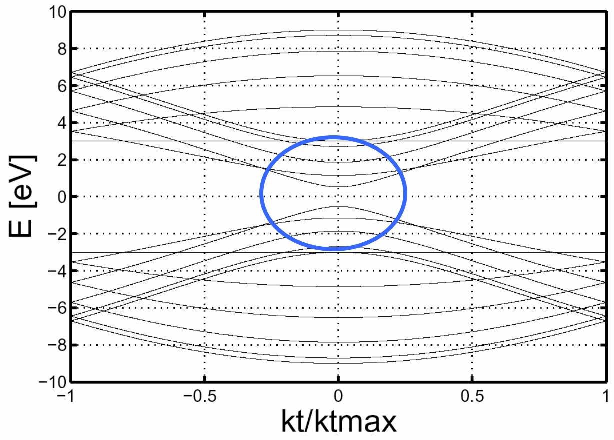
Acknowledgements

Theory: Mark Lundstrom, Supriyo Datta (Purdue)

Experiment: Hongjie Dai, Ali Javey (Stanford)

Carbon nanotubes





$$E(k) = \pm\left(\frac{E_G}{2}\right)\sqrt{1+(3kd/2)^2}$$

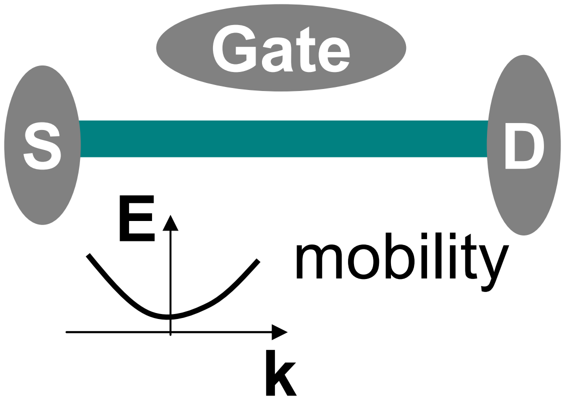
$$E_G \approx 0.8eV/d(\mathrm{nm})$$

McEuen, Fuhrer, Park, *IEEE Trans. Nanotech*., **1** , 78, 2002.

(see also: R. Saito, G. Dresselhaus, and M.S. Dresselhaus, *Physical Properties of Carbon Nanotubes*, Imperial College Press, London, 1998.)

Top-down and bottom-up view

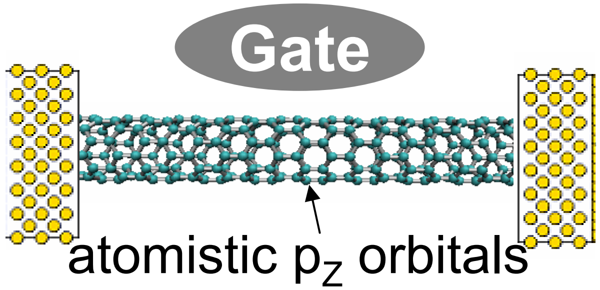
Top-down view



Semiclassical approach

applicable only when quantum effects not important

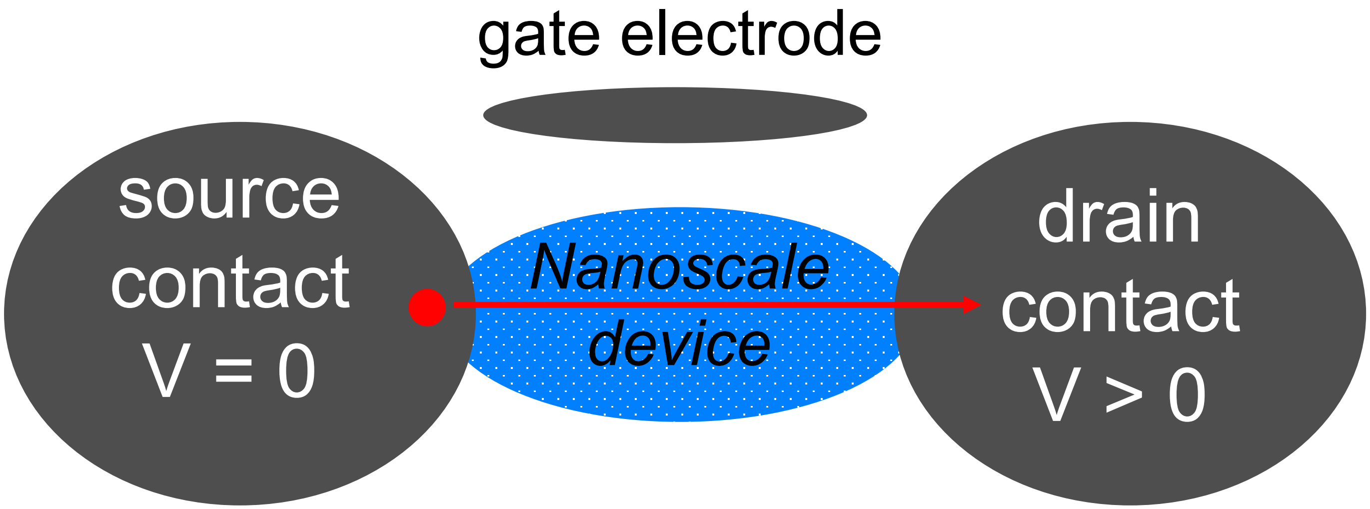
Bottom-up view



Quantum approach

- tunneling at M/CNT contacts
- tunneling and interference in the CNT

Quantum simulation for Nanoelectronics



Challenges in nanoscale device simulation:

1) description at an atomistic level
2) quantum description of open systems under bias
3) treatment of inelastic scattering

Our approach: the Green’s function formalism

Outline

1. Introduction
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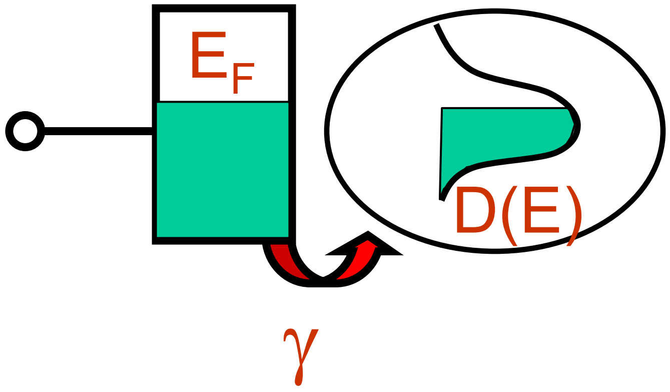
One contact

in-flow: $\frac{\gamma}{\hbar} D(E-U) f_0$

out-flow: $\frac{\gamma}{\hbar} N_E$



$$\frac{dN_E}{dt} = \frac{\gamma}{\hbar}[D(E-U) f_0(E-E_F) - N_E]$$

$$N = \int dE\, D(E-U) f_0(E-E_F)$$

Datta, *Quantum Transport Atom to Transistor*, Cambridge Univ. Press, 2005

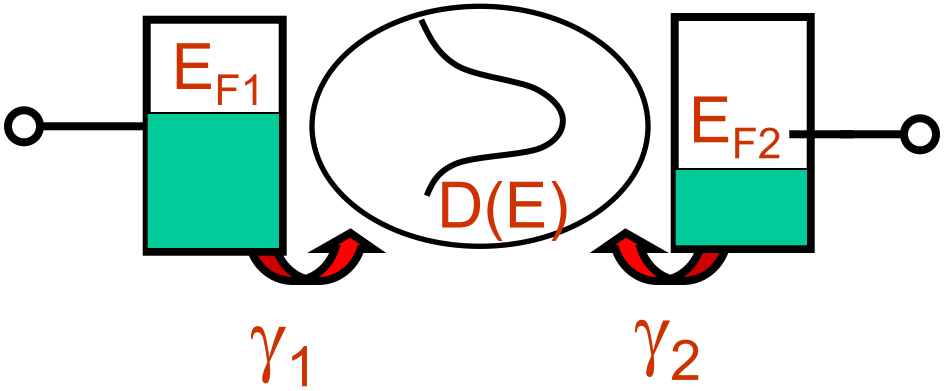
Two contacts

in-flow: $\frac{\gamma_1}{\hbar} D(E-U) f_1$ →

out-flow: $\frac{\gamma_1}{\hbar} N_E$ ←

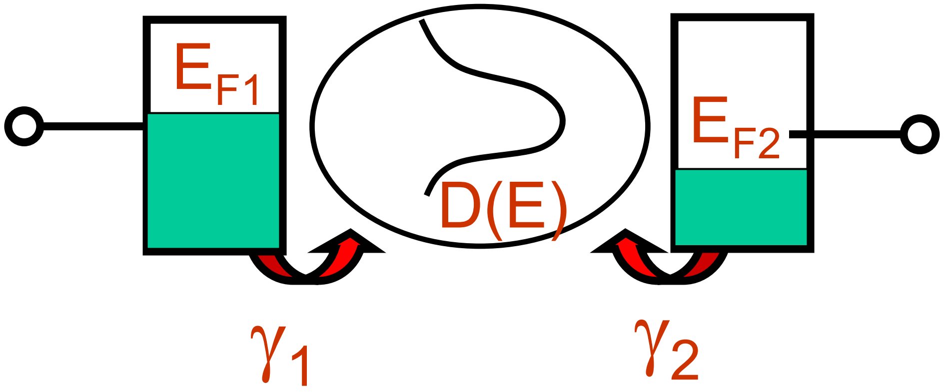
← in-flow: $\frac{\gamma_2}{\hbar} D(E-U) f_2$

→ out-flow: $\frac{\gamma_2}{\hbar} N_E$



$$\frac{dN_E}{dt} = \frac{\gamma_1}{\hbar}[D(E) f_1 - N_E] + \frac{\gamma_2}{\hbar}[D(E) f_2 - N_E]$$

Two contacts

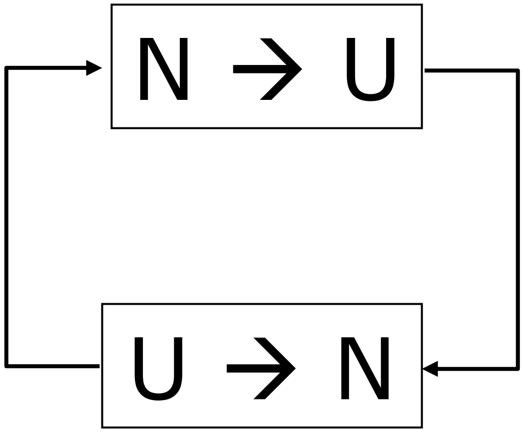


$$N = \int dE\ D(E-U)\left[\frac{\gamma_1 f_1 + \gamma_2 f_2}{\gamma_1 + \gamma_2}\right]$$

$$I = \frac{2q}{\hbar}\int dE\,D(E-U)\frac{\gamma_1\gamma_2}{\gamma_1+\gamma_2}\left[f_1 - f_2\right]$$

$$U = U_L + U_0(N - N_0)$$

“Poisson”



N → U

U → N

“Transport”

Rahman, Guo, Datta, Lundstrom, *IEEE Trans. Electron Dev.*, p. 1897 ,2003

Multiple levels

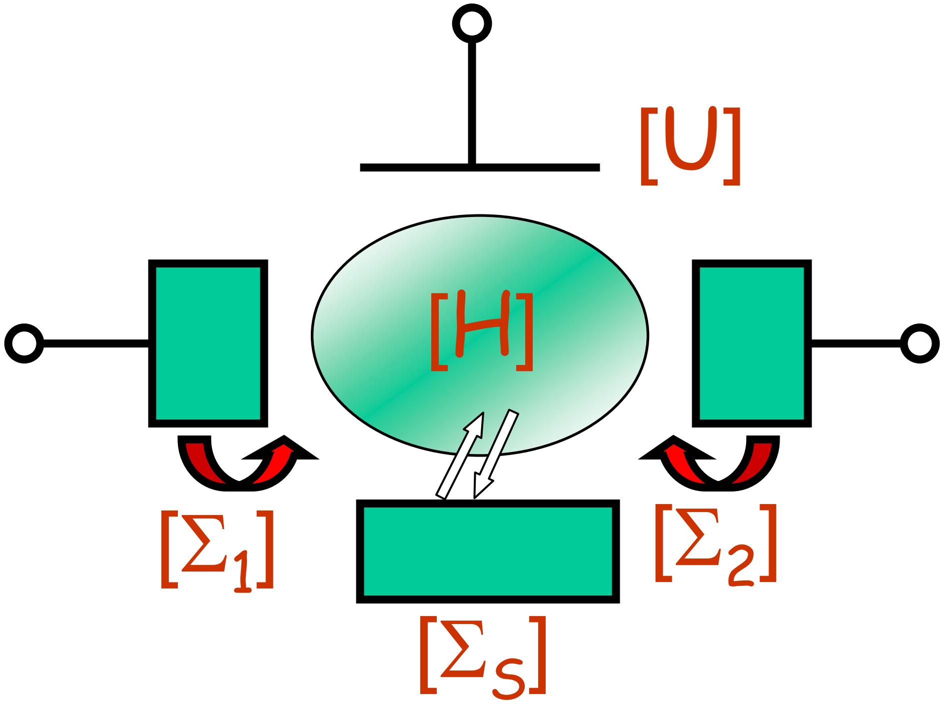
$$\varepsilon \rightarrow [H]$$

$$\gamma \rightarrow [\Gamma]$$

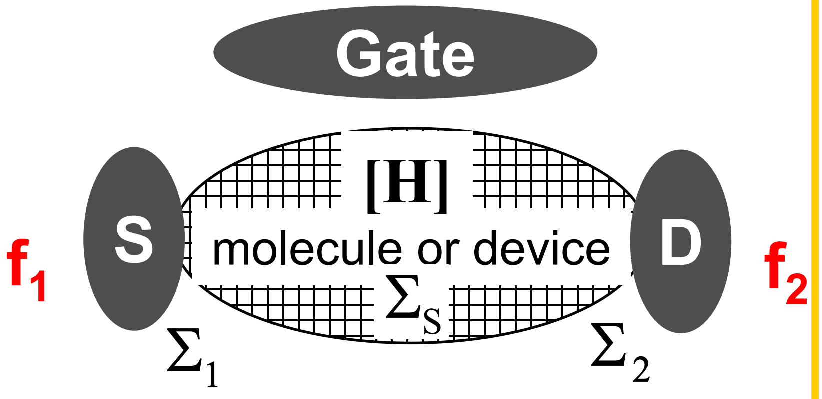
$$[\Sigma]$$

$$N \rightarrow [\rho]$$

$$G = [ES - H - \Sigma]^{-1}$$



Non equilibrium Green's Function (NEGF)



$$\mathbf{G} = \left[E\mathbf{I} - \underset{\uparrow\ \text{device}}{\mathbf{H}} - \underbrace{\Sigma_1 - \Sigma_2}_{\text{contacts}} - \underset{\uparrow\ \text{scattering}}{\Sigma_S}\right]^{-1}$$

Charge density (ballistic)

$$[\rho] = \int \left[A_1(E) f_1(E) + A_2(E) f_2(E)\right] \frac{dE}{2\pi}$$

Current

$$I_D = \frac{2q}{h} \int T(E)\big(f_1(E) - f_2(E)\big) dE$$

$$\mathrm{A}_{1,2}(E) = \mathrm{G}\ \ \Gamma_{1,2}\mathrm{G}^{+}$$

$$T(E) = \mathrm{Trace}[\Gamma_1 \mathrm{G}\ \ \Gamma_2 \mathrm{G}^{+}]$$

$$\Gamma_{1,2} = i[\Sigma_{1,2} - \Sigma^{+}_{1,2}]$$

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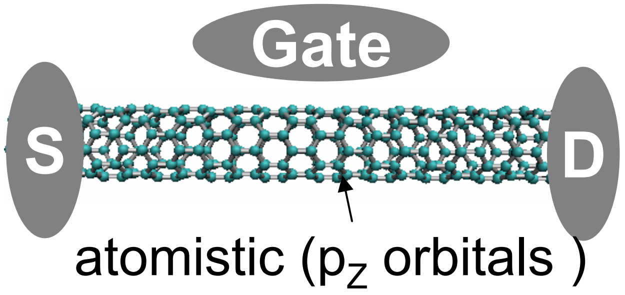
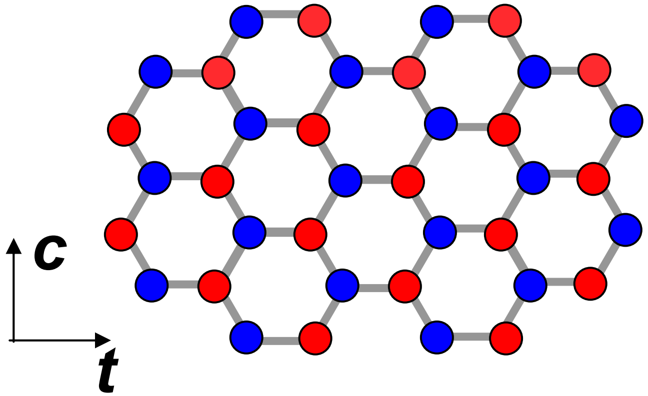
Real-space basis (ballistic)

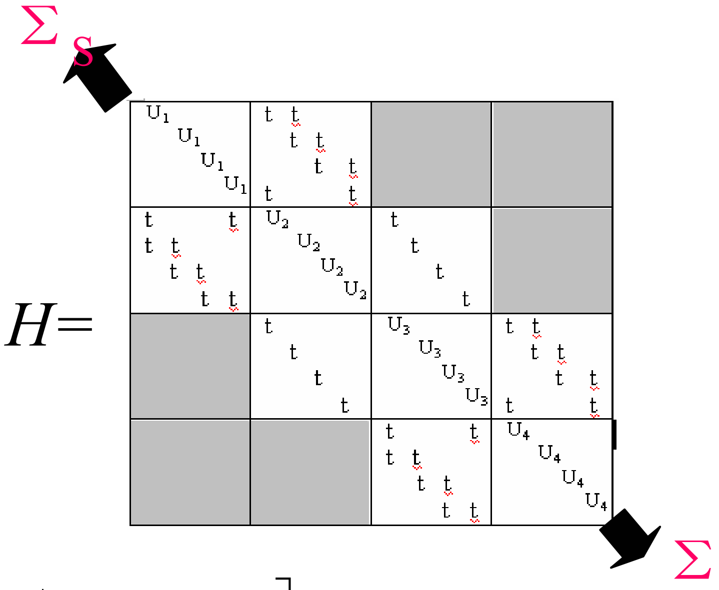


atomistic (p_Z orbitals)



(m, 0) CNT

$H=$



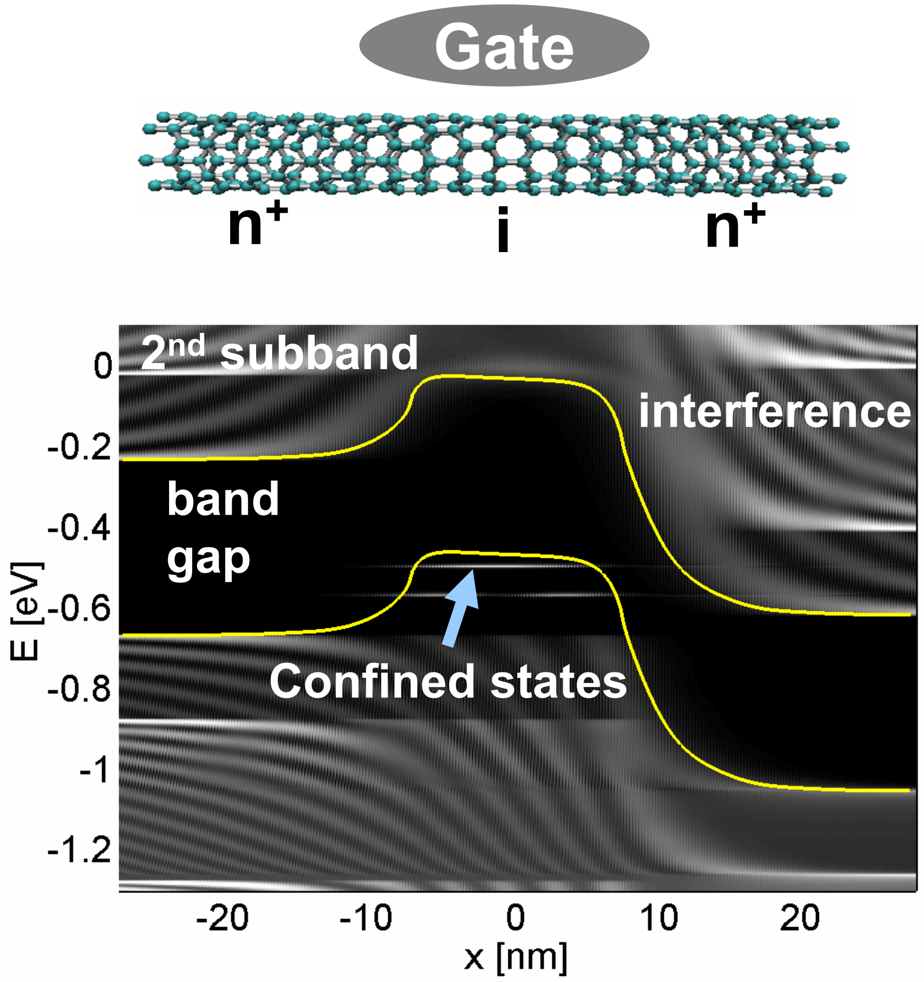
$$\Sigma_S = \begin{bmatrix} [\tau g_S \tau^+] & 0 & 0 & \\ 0 & 0 & 0 & \\ 0 & 0 & 0 & \\ & & & \ddots \end{bmatrix} \qquad \Sigma_D = \begin{bmatrix} \ddots & & & \\ & 0 & 0 & 0 \\ & 0 & 0 & 0 \\ & 0 & 0 & [\tau g_D \tau^+] \end{bmatrix}$$

$$G^r = [EI - H - \Sigma_S - \Sigma_D]^{-1}$$

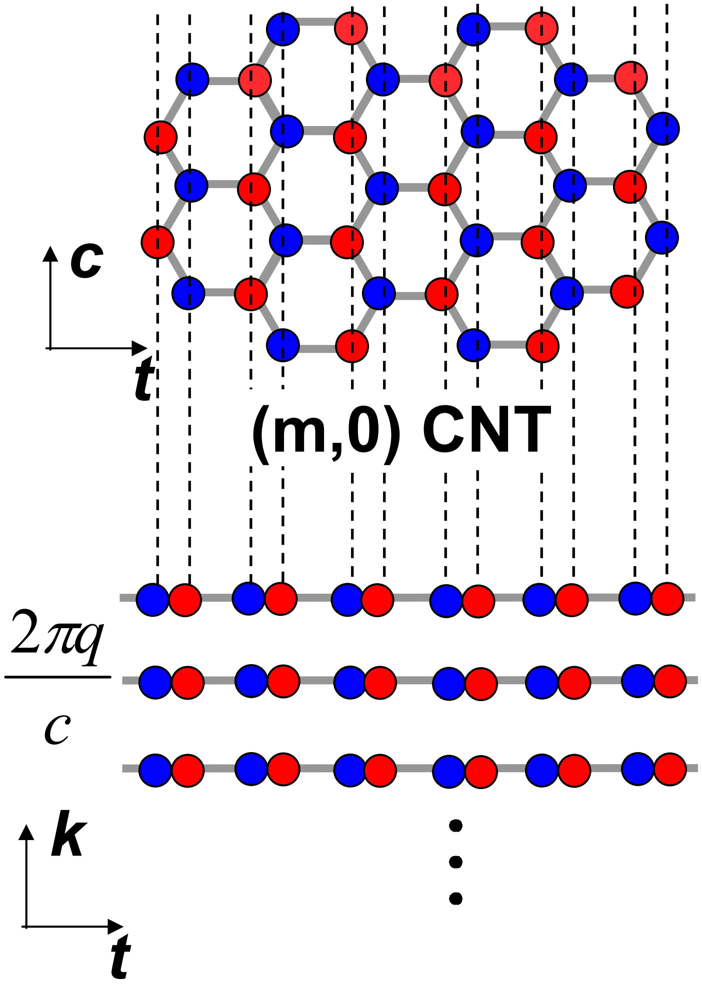
Recursive algorithm for G^r: $O(m^3N)$

Lake et al., JAP, **81**, 7845, 1997

Real-space results



Mode-space approach (ballistic)



$$k_q = \frac{2\pi q}{c}$$

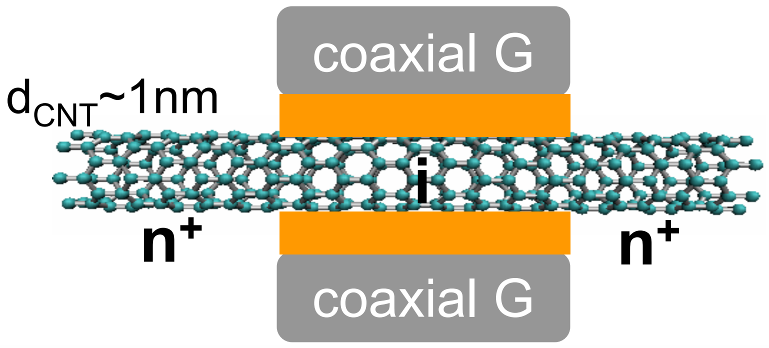
The *q*th mode

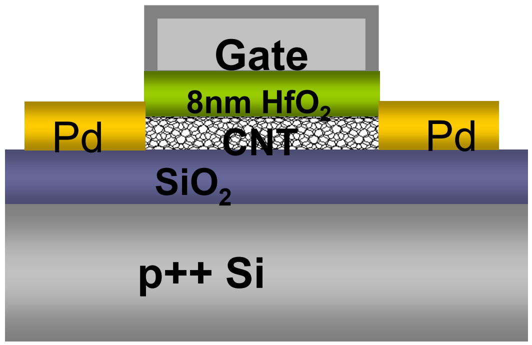
$$H_q = \begin{bmatrix} u_1 & b_q & & & \\ b_q & u_2 & t & & \\ & t & u_3 & \ddots & \\ & & \ddots & \ddots & b_q \\ & & & b_q & u_N \end{bmatrix}$$

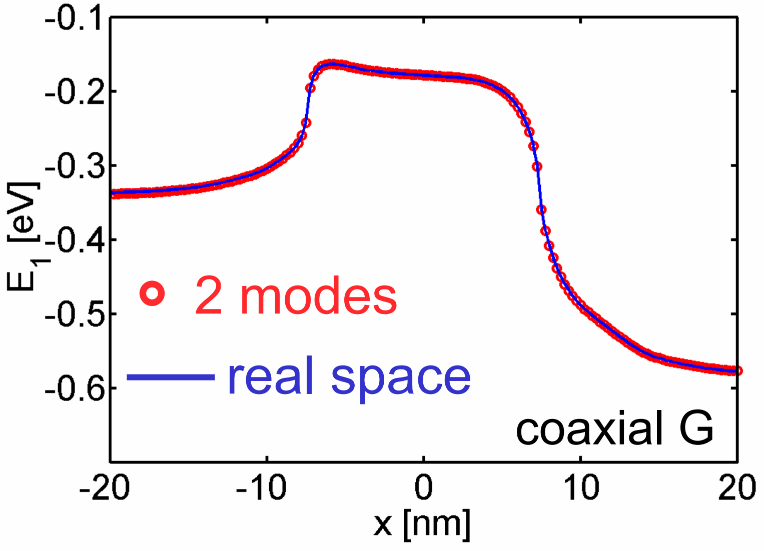
- **Σ_S (1,1) and Σ_D (N,N) analytically computed**
- **Computational cost: O(N)**

real space O(m^3N)

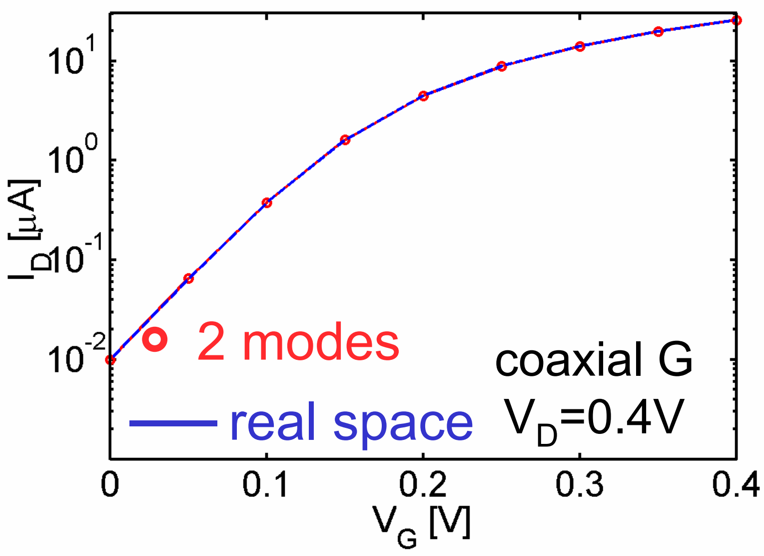
Mode-space results



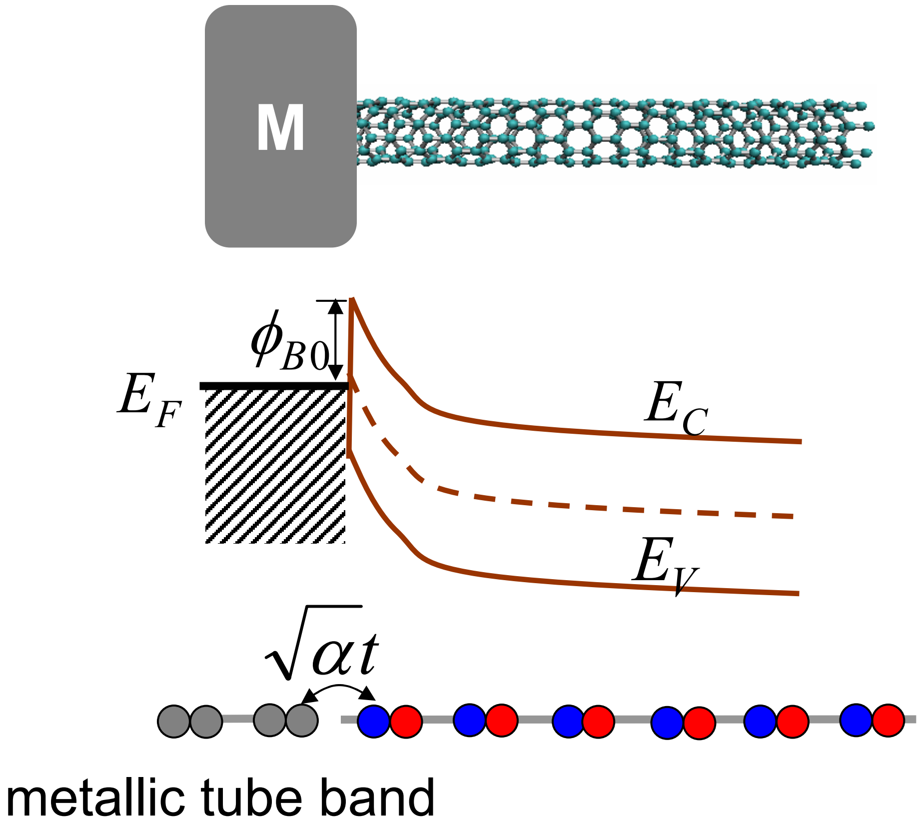




Conduction band profile (ON)



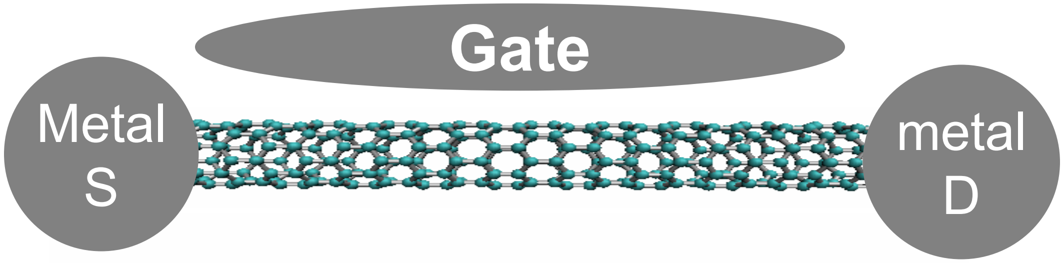
Treatment of M/CNT contacts

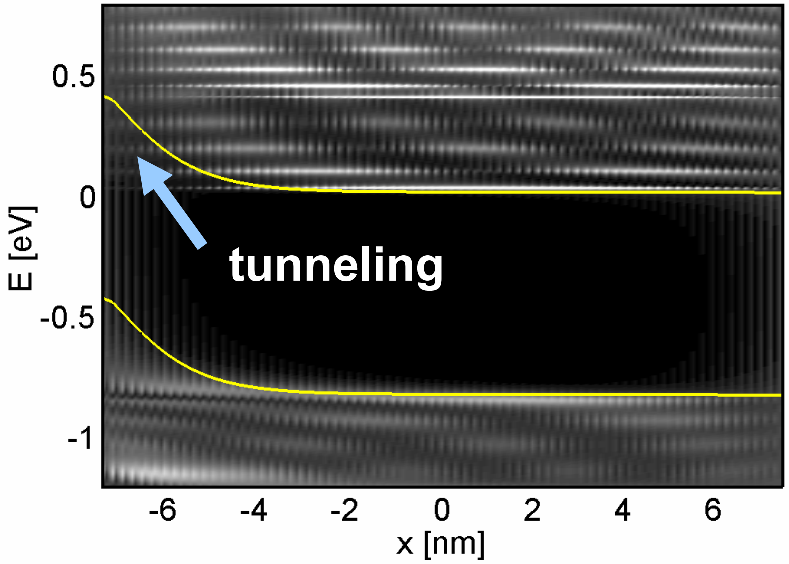


ϕ_{B0} : band discontinuity

$$\Sigma_m \approx \begin{bmatrix} -it\alpha & 0 & \\ 0 & 0 & \\ & & \ddots \end{bmatrix}$$

Treatment of M/CNT contacts

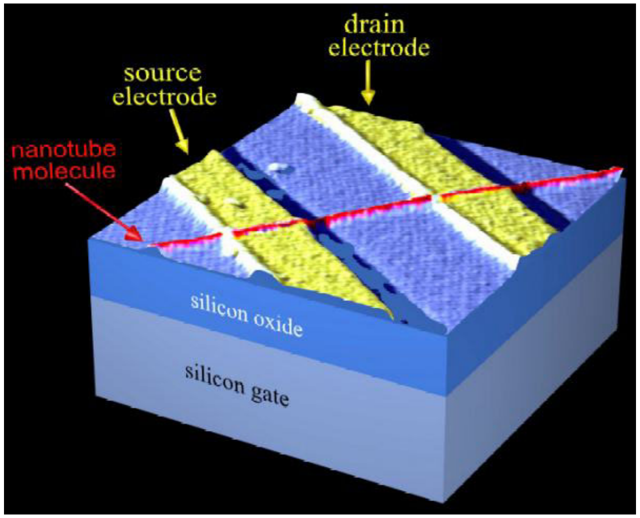




$V_D=V_G=0.4V$

Charge transfer in unit cell: Leonard et al., APL, **81**, 4835, 2002

3D Poisson solver



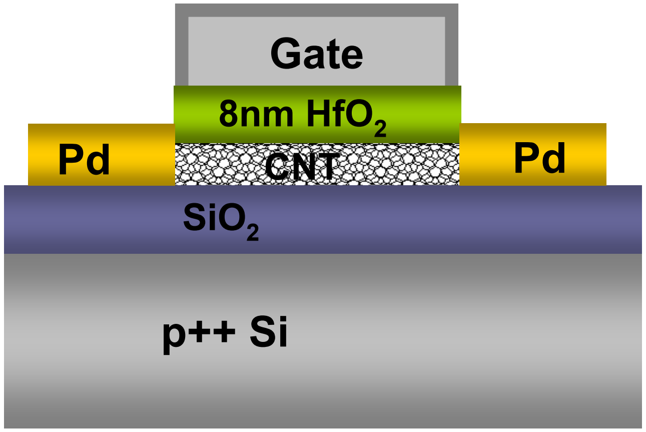
Method of moments:

$$V(\vec{r}) = \int K(\vec{r} - \vec{r}\,')\rho(\vec{r}\,')d\vec{r}\,'$$

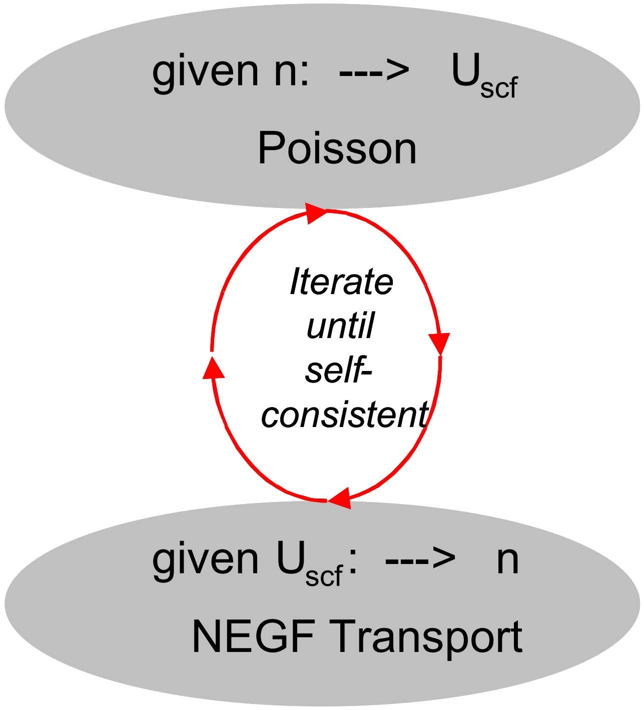
Electrostatic kernel:

$$K(\vec{r} - \vec{r}\,')$$

$K(\vec{r} - \vec{r}\,')$ for 2 types of dielectrics available in Jackson, *Classical Electrodynamics, 1962*



Numerical techniques



given n: ---> U_{scf}

Poisson

Iterate until self-consistent

given U_{scf}: ---> n

NEGF Transport

- Non-linear Poisson
- Recursive algorithm for

$$G(E) = [EI - H - \Sigma_S - \Sigma_D]^{-1}$$

- Gaussian quadrature for doing integral
- Parallel different bias points
- ~20min for full I-V of a 50-nm CNTFET

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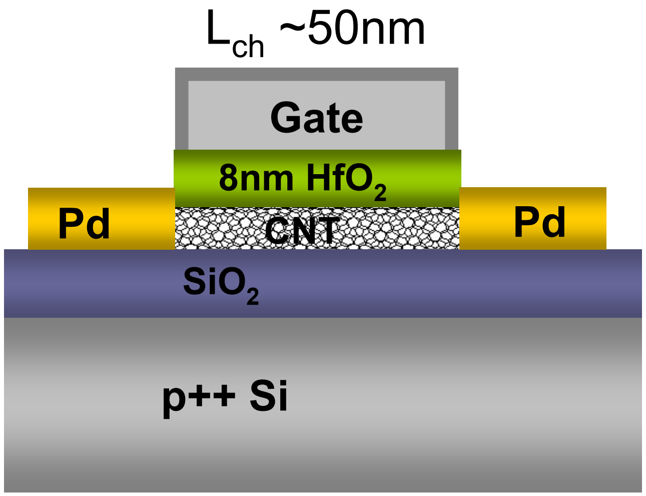
Device issues

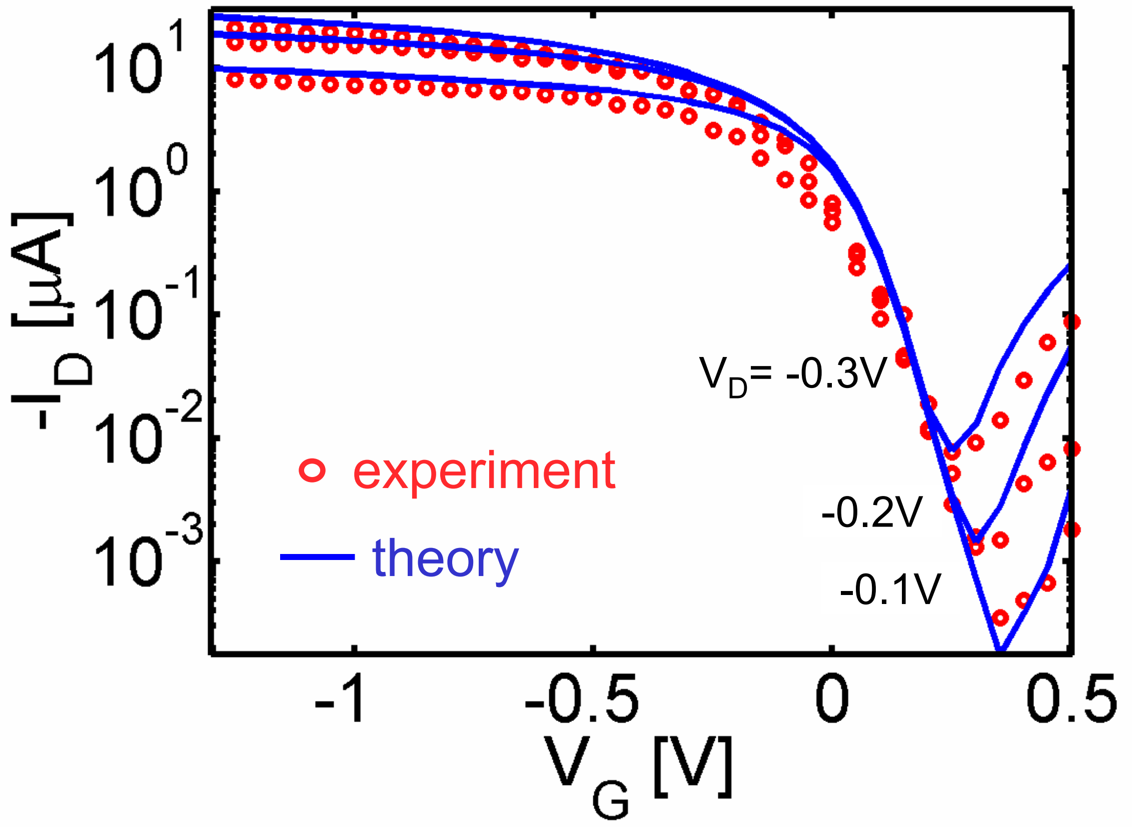
nanotube diameter ~1.7 nm



Javey et al, Nano Lett., 2004

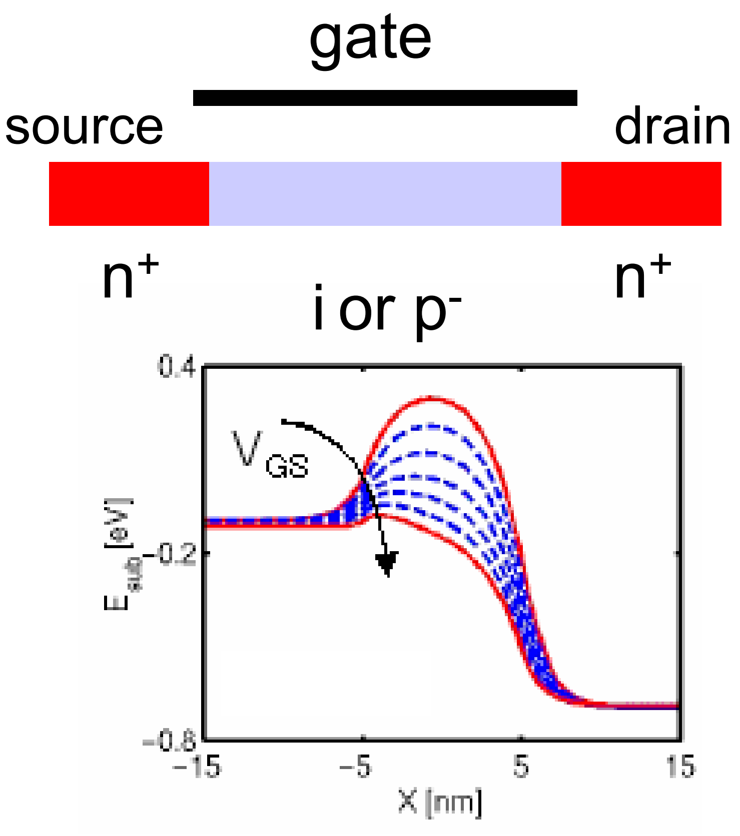
1) Can we model and understand I-V?
2) How close to the ballistic limit?
3) What is the role of scattering?
4) How to optimize I_{ON} ?
5) How to reduce I_{off} ?
6) How to compare to Si MOSFETs?

Modeling I_D-V_G

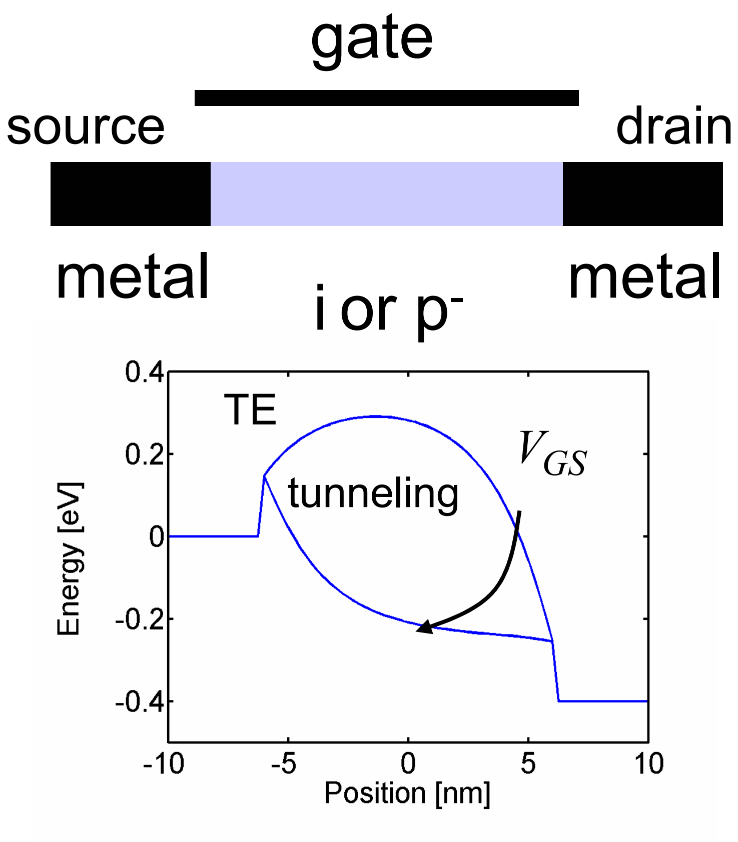


SB height: $\phi_{Bp}=0$, d_{CNT} ~1.7nm $R_S=R_D$~1.7KΩ

Two kinds of transistors



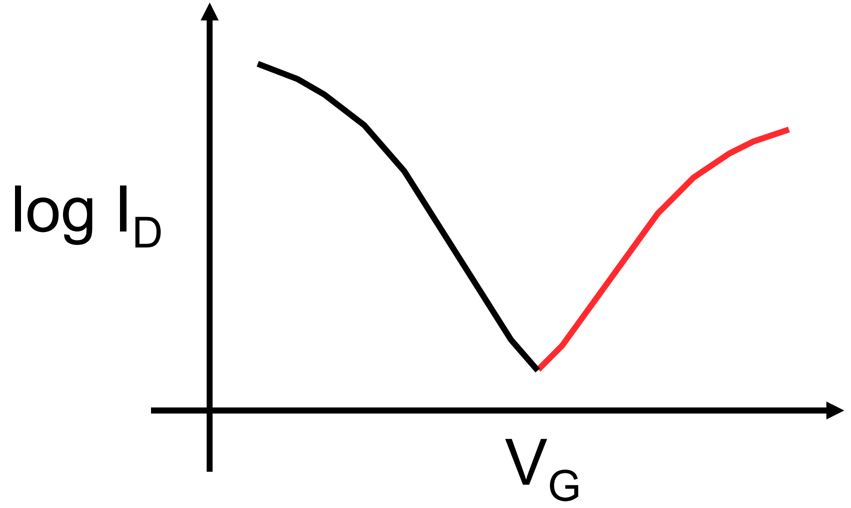
MOSFET



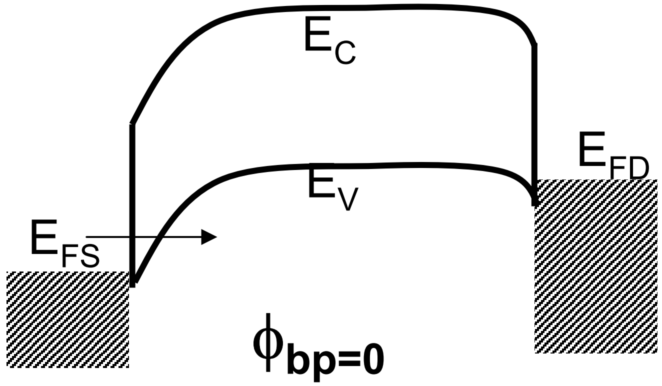
SBFET

Carbon nanotubes as Schottky barrier transistors
Heinze et al, *PRL*, **89**, 106801,2002

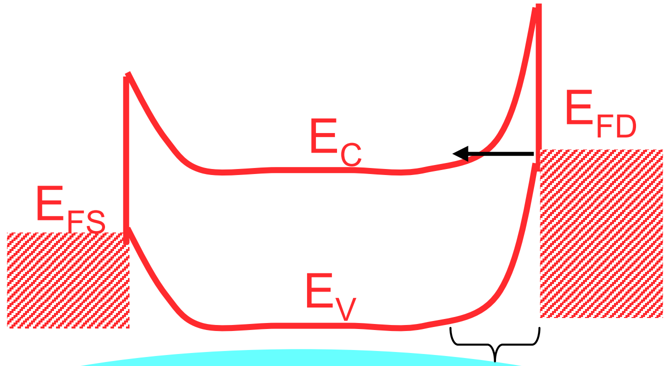
Ambipolar conduction (thin oxide)



hole conduction at low V_G



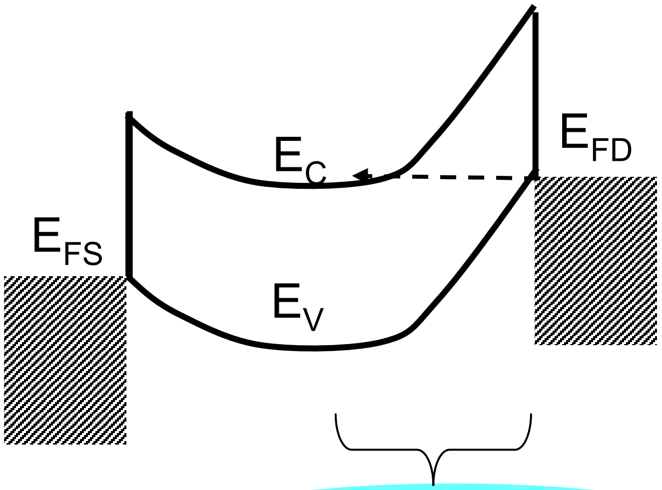
electron conduction at high V_G



barrier thickness set by t_{ins}
(geometric screening)

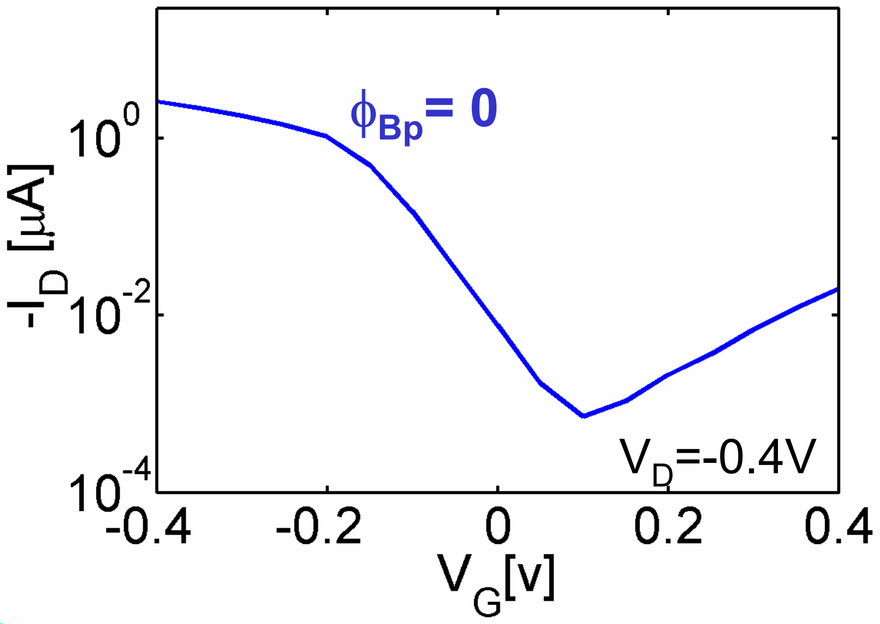
Thick oxide

opaque barrier for electron tunnelinng



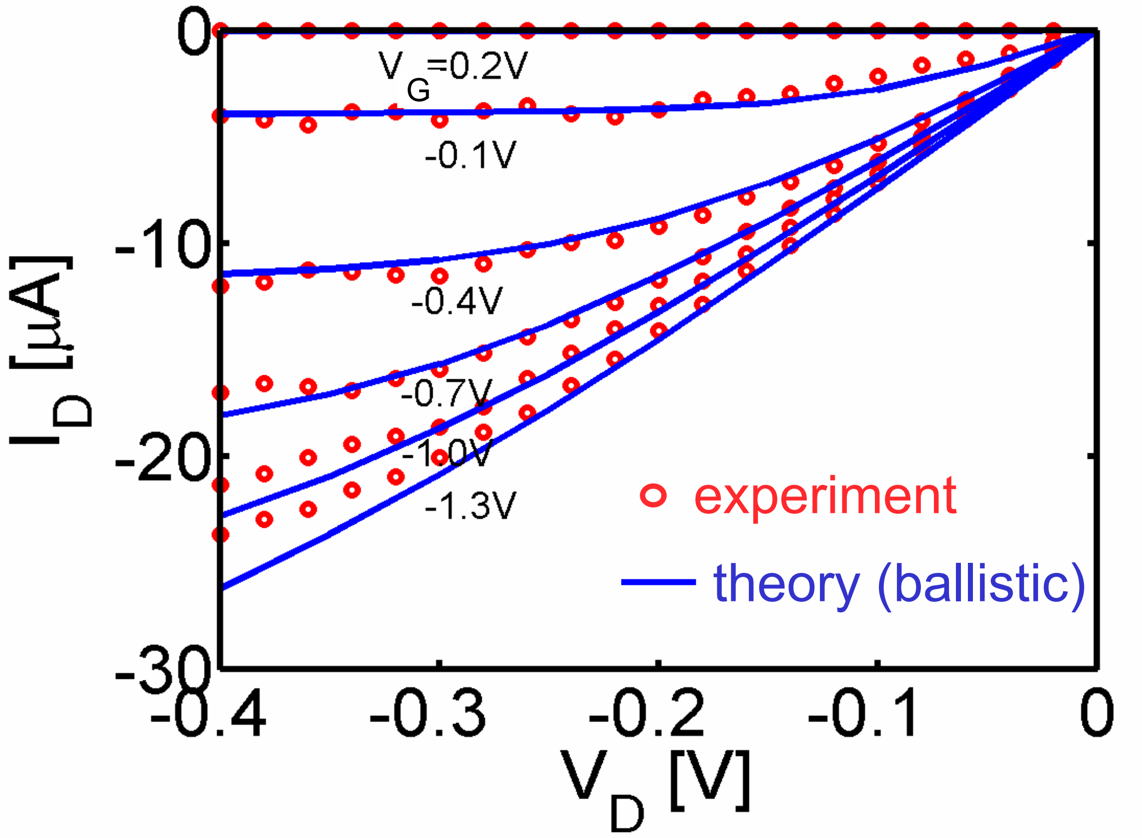
barrier thickness set by t_{ins}
(geometric screening)

t_{ox} = 40 nm



Guo, Datta and Lundstrom, *IEEE Trans. ED*, **51**, 172, 2004

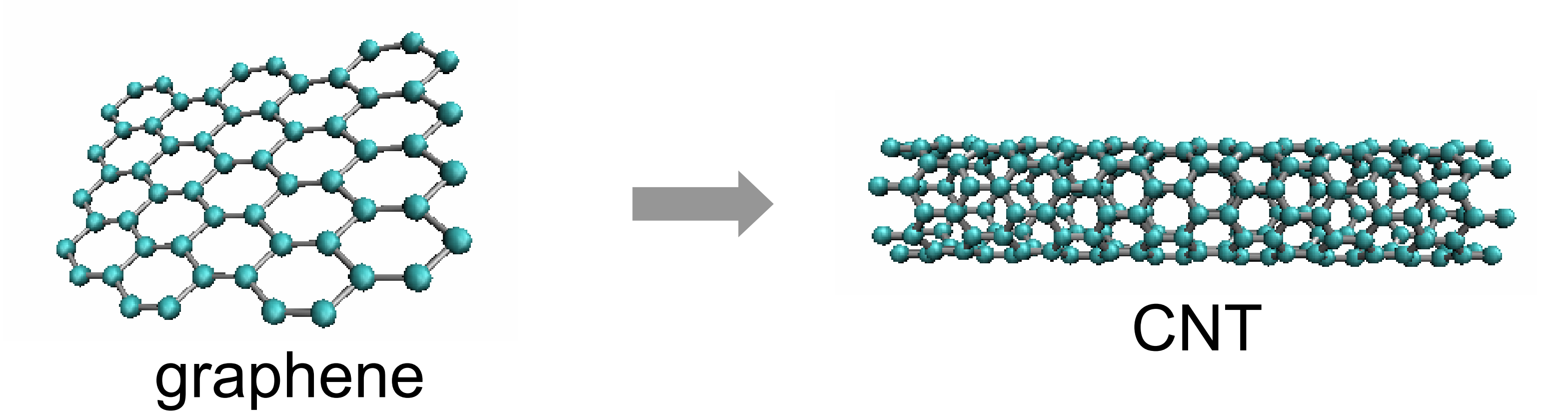
How close to ballistic limit?



SB height: $\phi_{Bp}=0$, $d_{CNT}\sim 1.7$nm, $R_S=R_D\sim 1.7\text{K}\Omega$

⇨ Deliver near-ballistic DC on-current

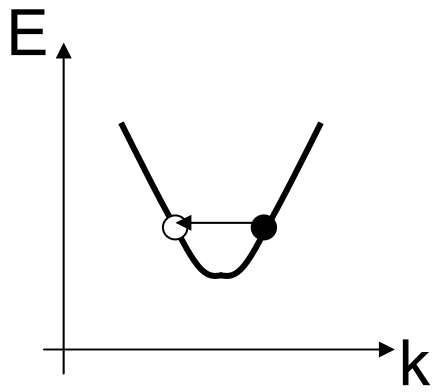
No surface roughness scattering in CNTs



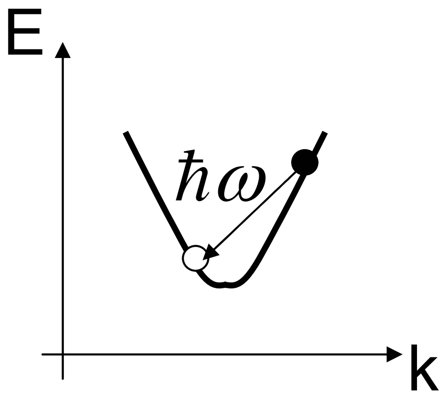
Phonon scattering dominates in CNTs

Yao, Kane, and Dekkeer, *Phys. Rev. Lett.*, **84**, 2941, 2000

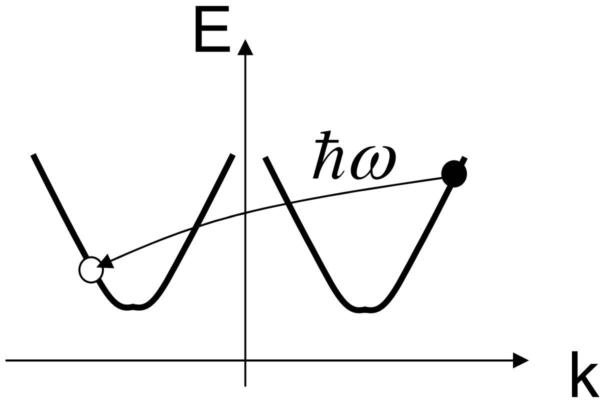
Phonon scattering in CNTs



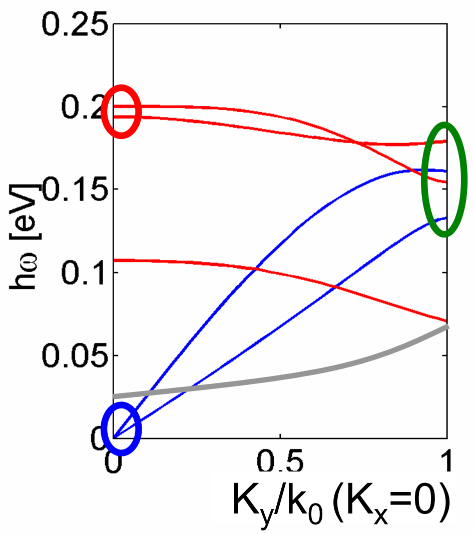
● **AP**



● **OP(intra.)**



● **OP (intervalley)**



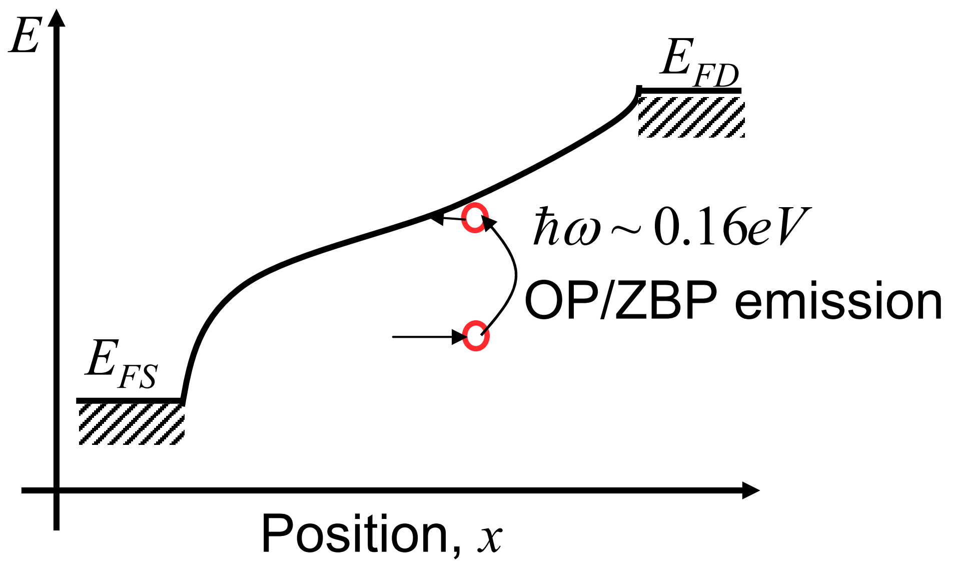
AP: long mfp (λ_1^{high}~1μm)

OP: short mfp (λ_2^{high}~10nm)

Javey, Guo, Paulsson et al., *Phys. Rev. Lett.*, **92**, 106804, 2004

Park, Rosenblatt, Yaish et al.,Nano Lett., **4**, 517

Small effect of OP scattering

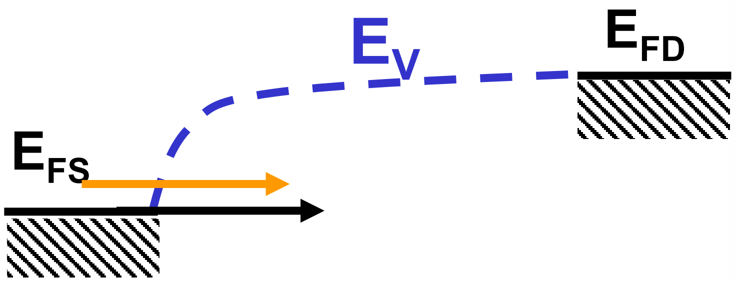


⇨ Deliver near-ballistic DC on-current

confirmed by a separate Monte-Carlo simulation

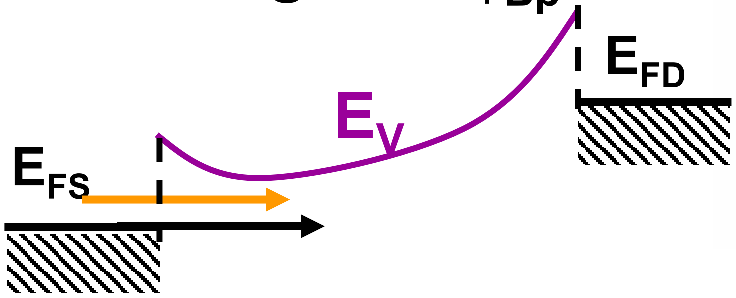
How close to the ballistic limit?

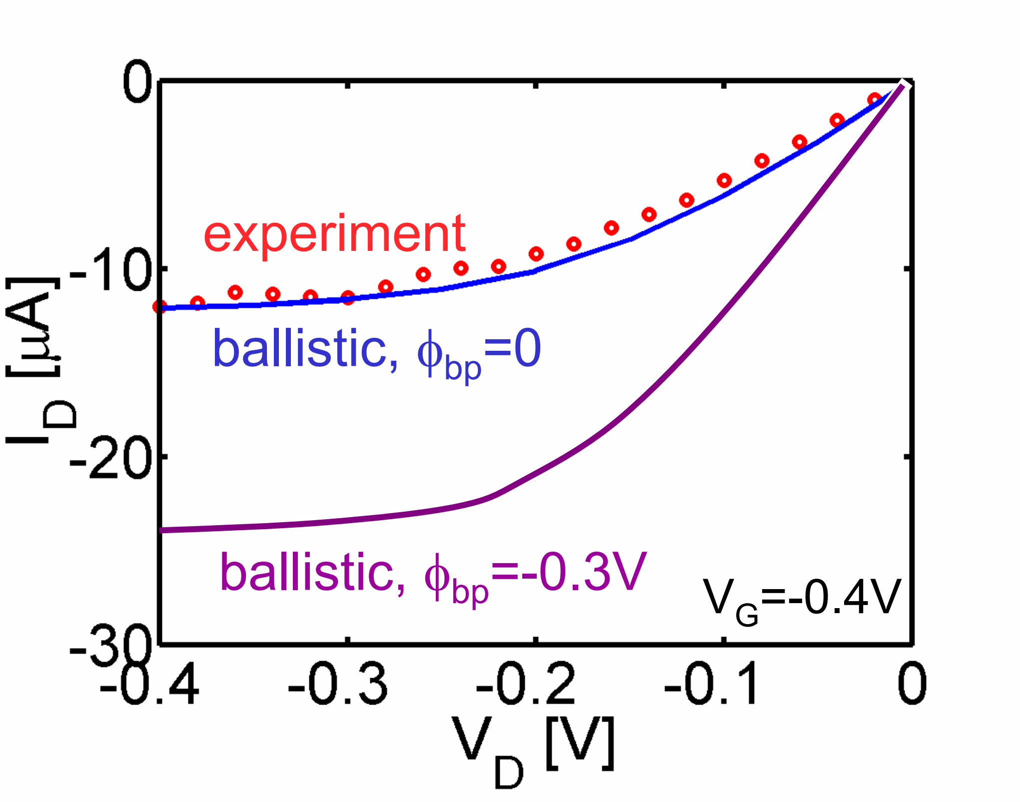
$\phi_{Bp} = 0$



⇨ **zero SB still limits I_D**

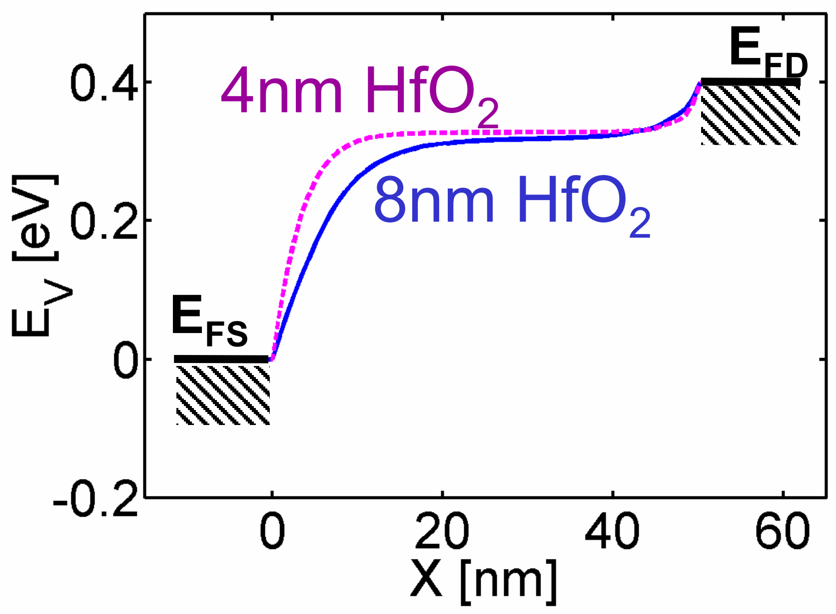
negative ϕ_{Bp}

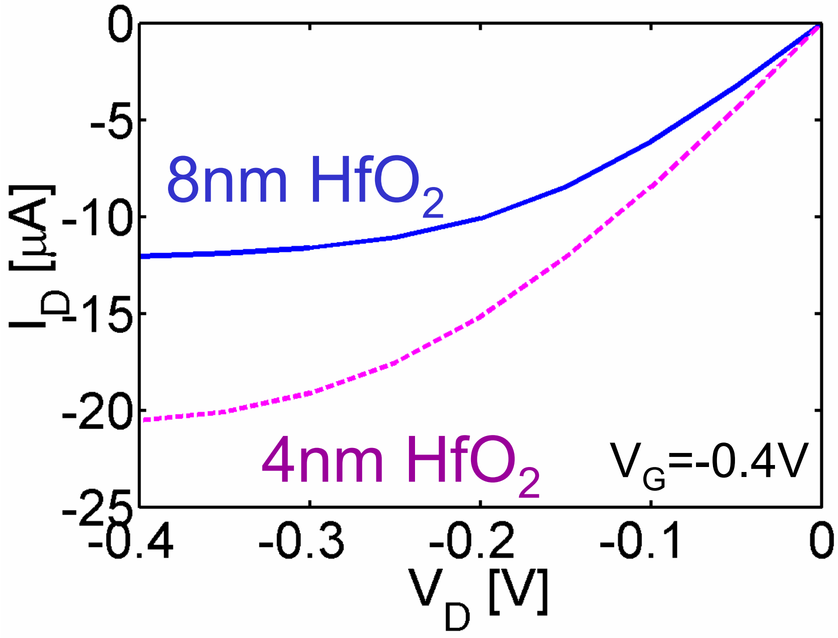




Guo and Lundstrom,
IEEE TED, **49**,1897, 2002 (silicon)

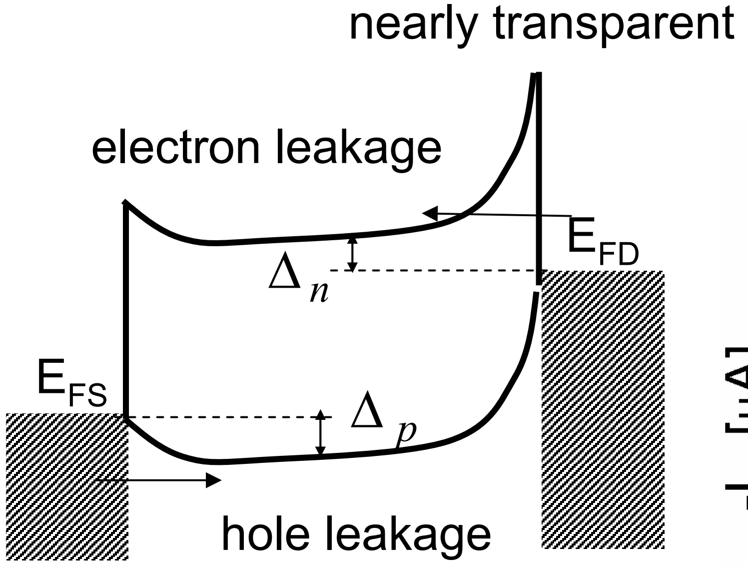
Improving I_{ON}: Scaling t_{ins}





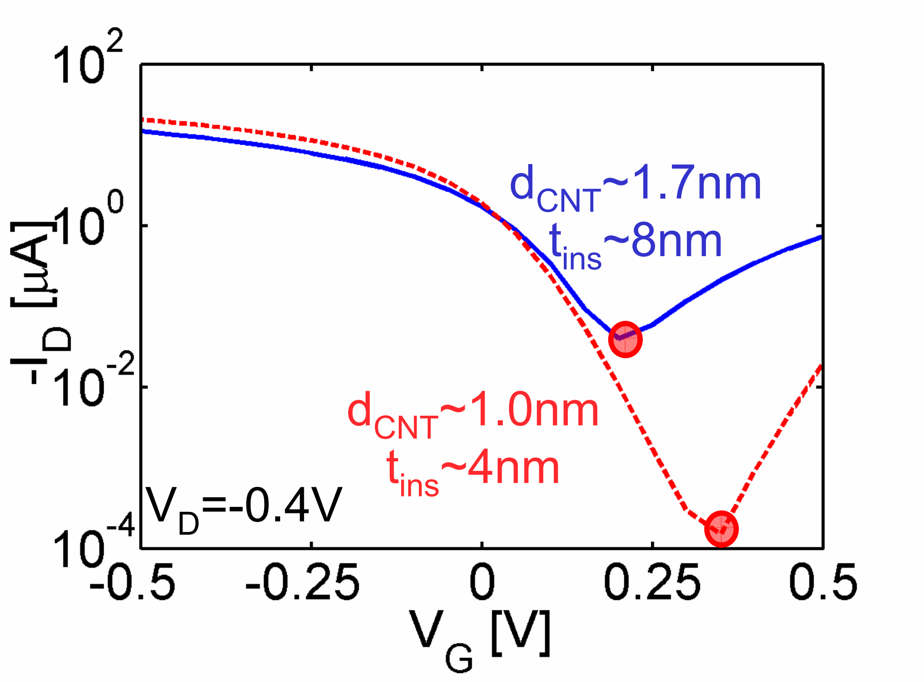
barrier thickness set by t_{ins}
(geometric screening)

Reduce I_{off} for thin t_{ins}



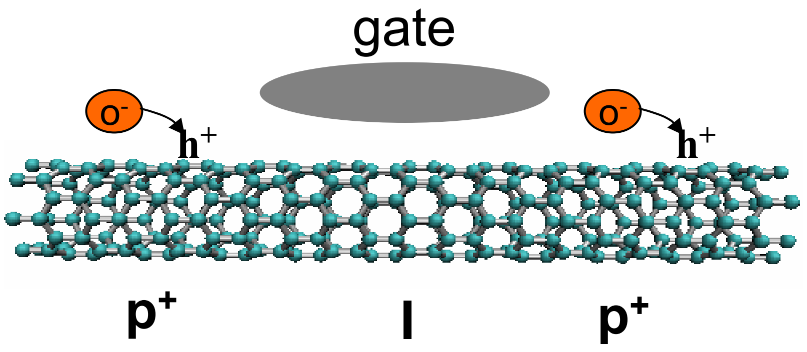
$$\Delta_n \sim \Delta_p \sim \frac{E_g - eV_D}{2}$$

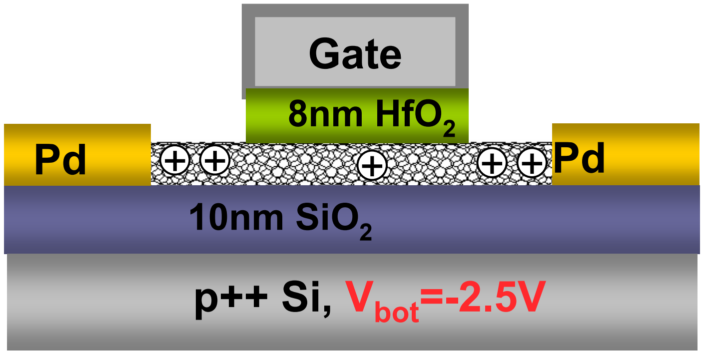
E_g~0.8eV/d(nm)



small d_{CNT} reduces I_{min}

Reduce I_{off} using MOSFET-like structure





chemical S/D doping

Chen et al., IEDM Tech Dig, 2004

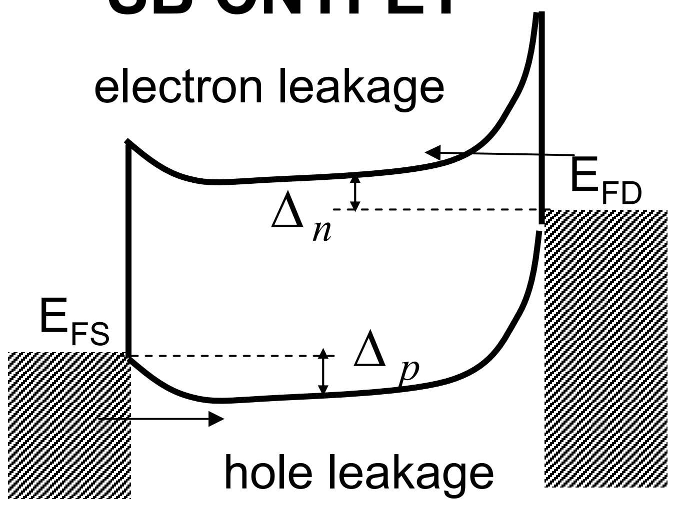
Javey et al., Nano Lett., 2005

electrical S/D doping

Appenzeller et al, PRL, 2004

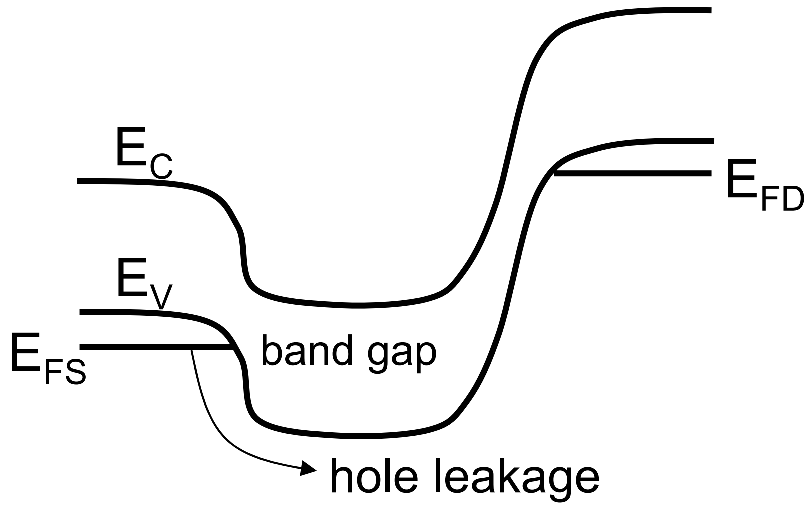
Reduce I_{off} using MOSFET-like structure

SB CNTFET



ambipolar $\Delta_n \sim \Delta_p \sim \dfrac{E_g - eV_D}{2}$

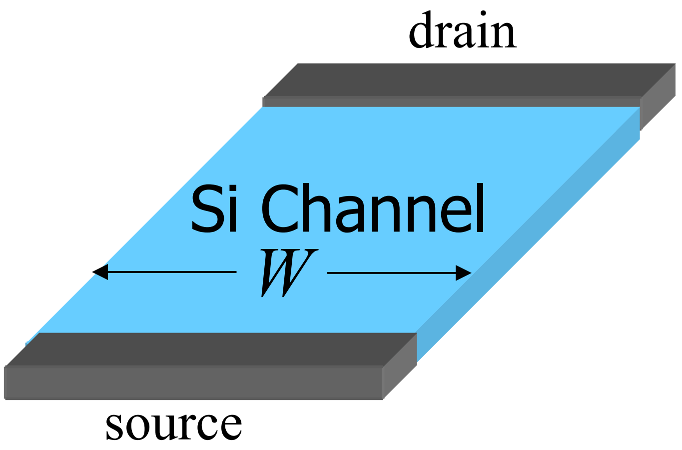
MOSFET-like CNTFET



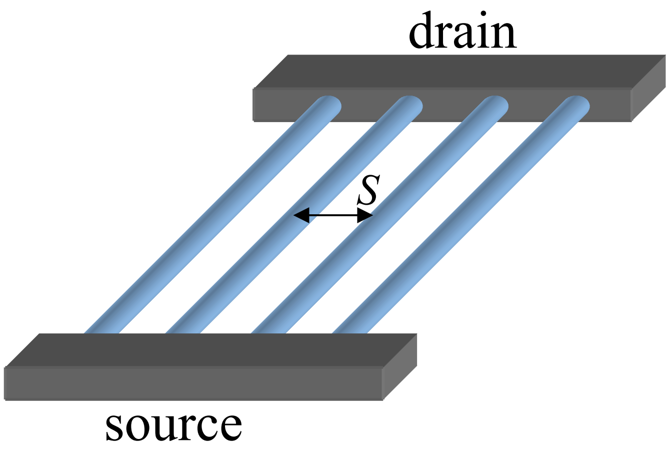
unipolar $\Delta_p \sim E_g$

Suppressed ambipolar conduction

How to compare to Si MOSFET?



Si MOSFETs



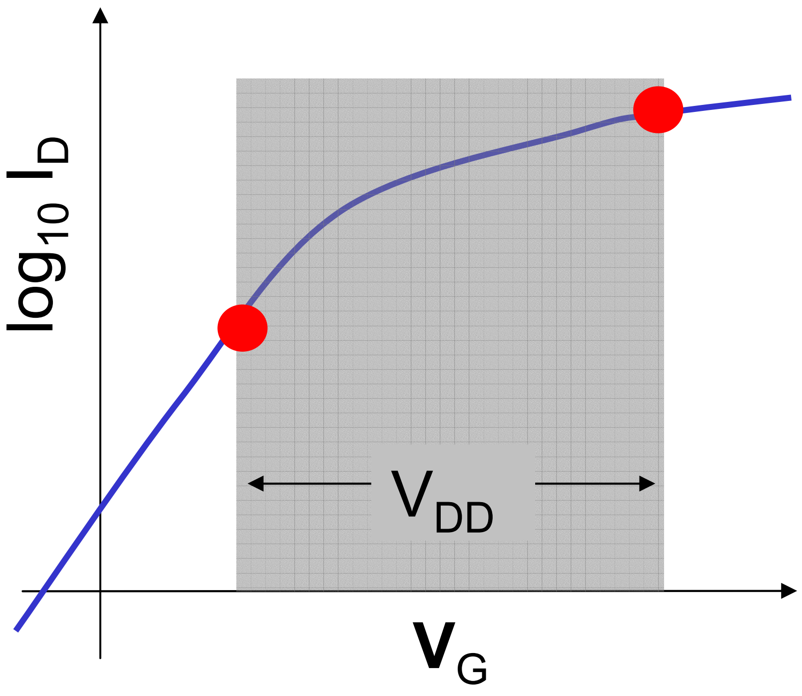
CNT array FETs

Key device metrics:

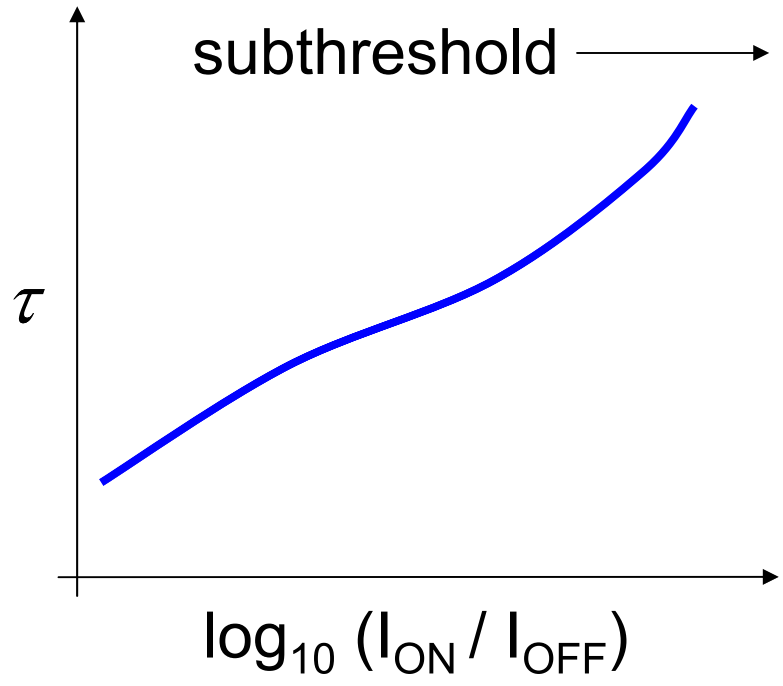
$$I_{ON}/I_{OFF}$$

$$\tau = C_G V_{DD}/I_{ON}$$

τ vs. I_{ON}/I_{OFF} technique

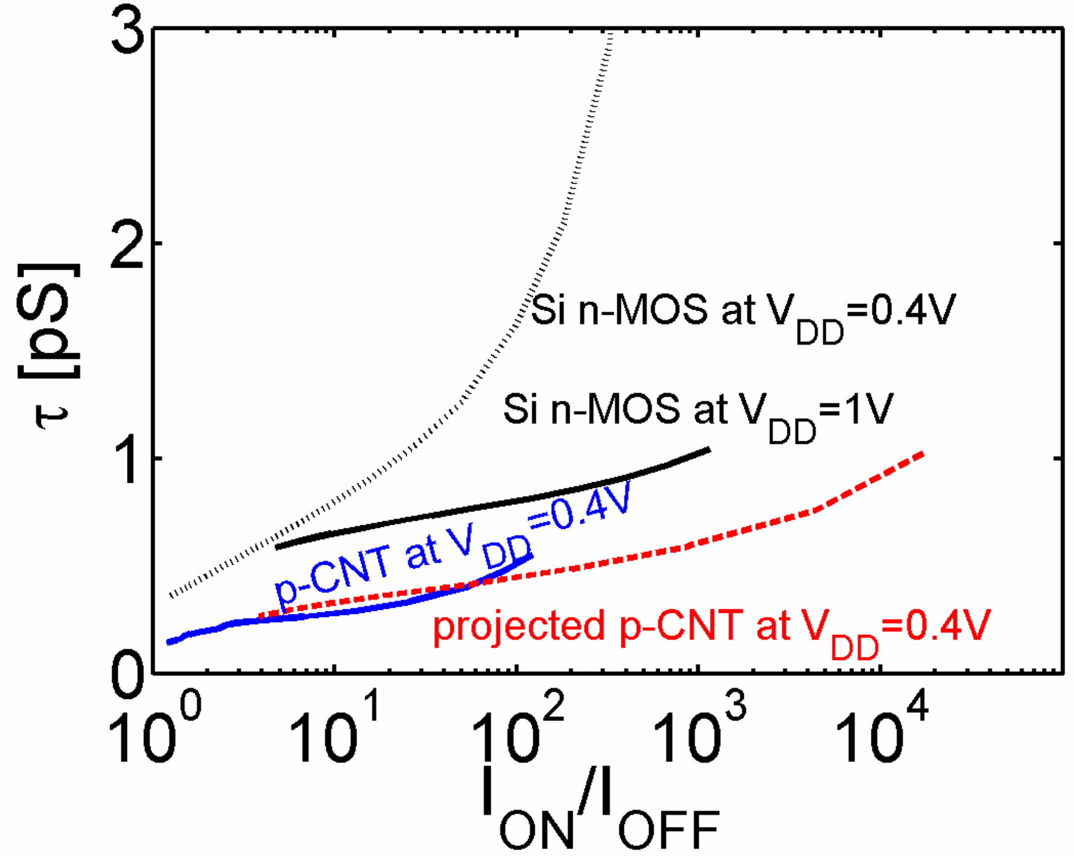


Control of V_T shifts the window



$$\tau = C_G V_{DD} / I_{ON}$$

Compare to 90nm Si MOSFETs



90nm Si n-MOS data from Antoniadis and Nayfeh, MIT

Outline

1. Introduction
2. NEGF formalism
3. Simulation Approach
4. Device Analysis
5. Summary

Summary: Simulation Approach

Quantum Transport (NEGF formalism)

- Atomistic description
- Non-equilibrium transport
- Inelastic scattering

Three dimensional Electrostatics

- Method of moments

Computational techniques

- recursive algorithm
- mode-space approach
- parallel simulation

Summary

1) I-V can be modeled and explained.
2) The CNTFET delivers near-ballistic I_{ON}
3) Scaling t_{ins} and using high-κ improves I_{ON}
4) Thin t_{ins} results in ambiploar conduction
5) Using small d_{CNT} tube or MOSFET-like structure suppresses ambipolar conduction
6) The CNTFET performance is promising

Outlook:

Transistors

- 3D electrostatics
- phonon scattering
- Advanced transistor structures
- AC characteristics

New devices

- CNT optoelectronic devices
- CNT-based nanosensors