Quantum Capacitance Effects In Carbon Nanotube Field-Effect Devices

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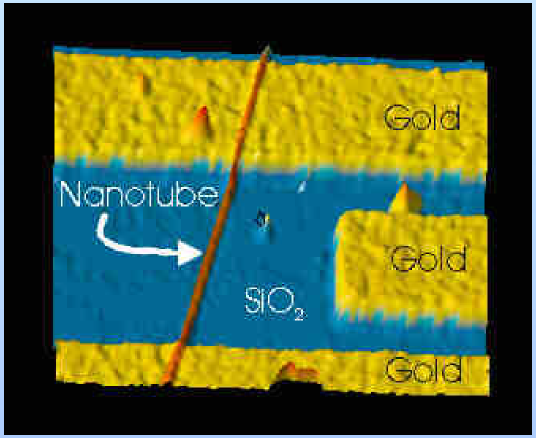
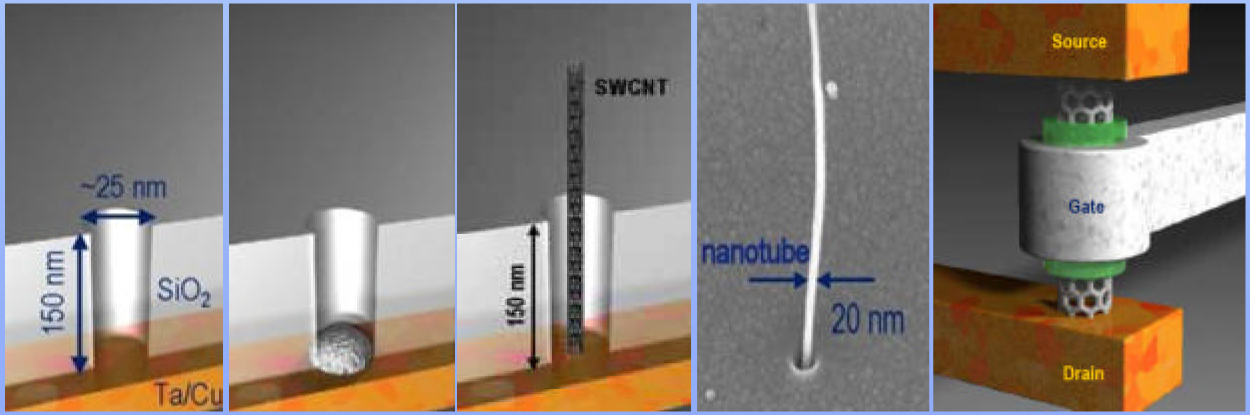
Devices based on field effect (CNTFET)



Planar geometry top/bottom gate (IBM)

- ULSI Devices
- Quasi-1D coherent transport over long distances
- Si integrable technology



Vertical Geometry coaxial gate (Infineon)

gDFTB

Green's functions Density Functional Tight-Binding

(A.Pecchia, L.Latessa, A.Di Carlo)

Atomistic simulations:

Quantum treatment

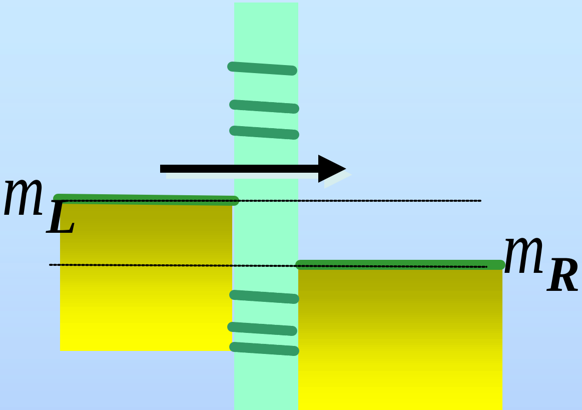
$$\hat{H} y_k(\vec{r}) = E_k y_k(\vec{r})$$

$$E[n(\vec{r})] = T_0[n(\vec{r})] + E_{Hartree}[n(\vec{r})] + E_{XC}[n(\vec{r})]$$

Approximated DFT:

$$E^{(2)} = \sum_i n_i \langle y_i | H_0 | y_i \rangle + \frac{1}{2} \sum_{m,n} g_{mn} \Delta q_m \Delta q_n + E^{rep}$$

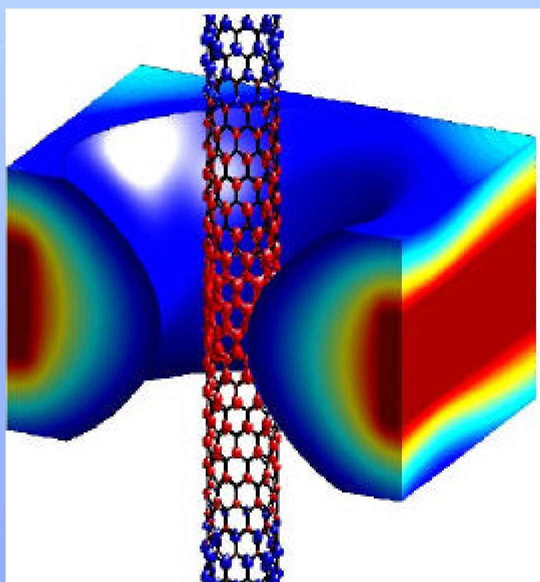
NEGF Extention



$$r_{mn} = \frac{1}{2p i}\int dE \; G^{<}_{mn}$$ Density Matrix

$$\Delta q_m = q_m^0 - \sum_n r_{mn} S_{mn}$$ Mullikan Charges

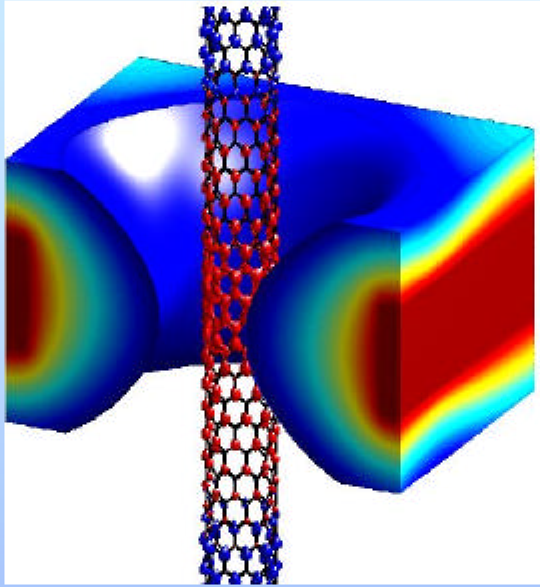
$$d n \rightarrow \nabla^2 dV_H = -4p d n \rightarrow dH \rightarrow dG^{<} \rightarrow dn'$$ SCC loop



A. Pecchia, A. Di Carlo, **Rep Prog Phys 67**, 1-65 (2004)

3D Poisson Multigrid

$$\vec{\nabla}\left(e_r(\vec{r})\vec{\nabla}V(\vec{r})\right) = -4p\,r(\vec{r})$$

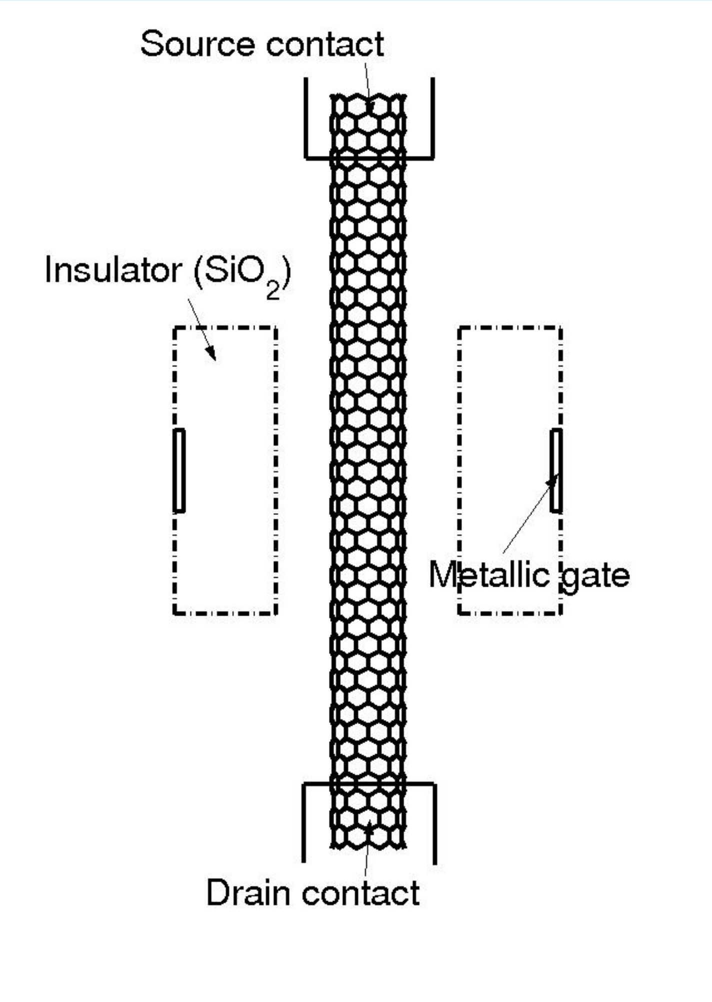


The cylindrical gate is added as an appropiate Dirichlet boundary condition

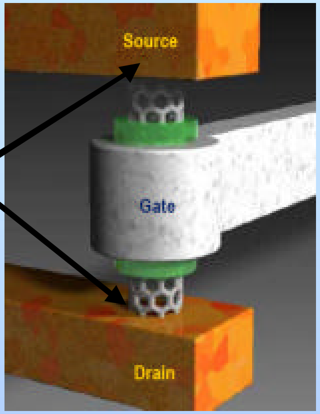
$\vec{r} \in$ Metal Gate $\longrightarrow$ $C_{ii} = C_i = 0: \quad C(\vec{r})V(\vec{r}) = r(\vec{r})$

$\vec{r} \in$ Insulating dielectric and CNT $\longrightarrow$ $C_i = C = 0: \quad C(\vec{r})\nabla^2 V(\vec{r}) = r(\vec{r})$

Coaxially gated CNTFET



Working mechanisms:



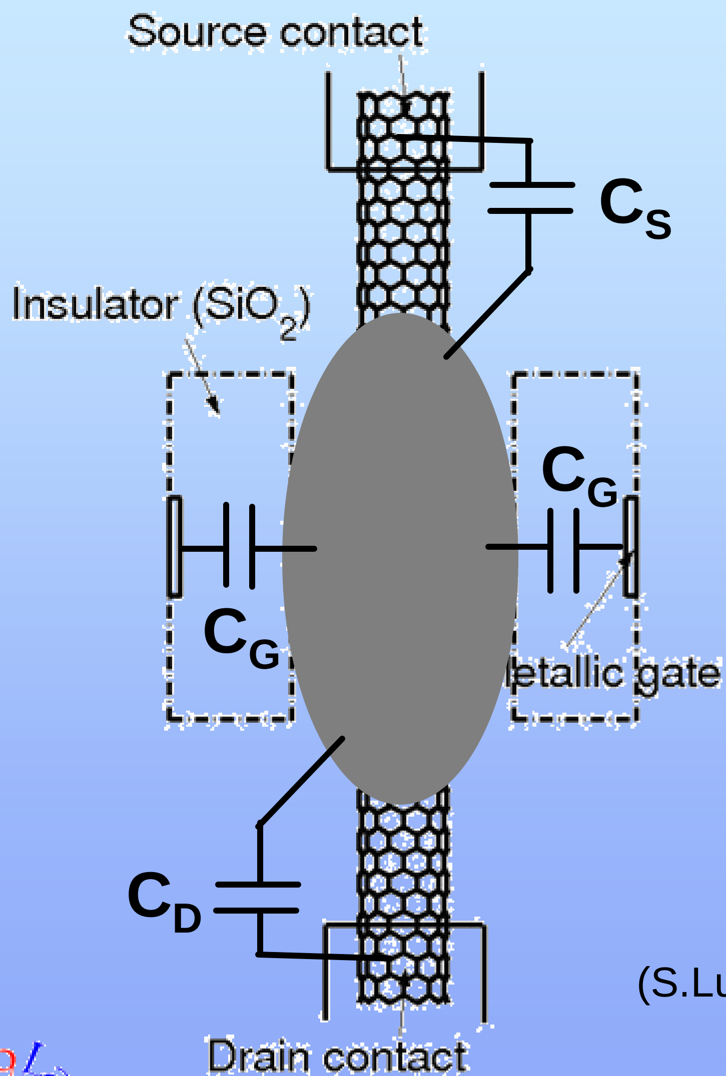
- Schottky barrier modulation at the contacts

- local modulation of channel conductance

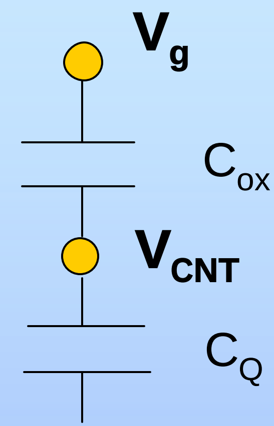
Model:

- semiconducting CNT(10,0)
- neglect Schottky barrier
- Charge injection from p-doped CNT contacts

CNTFET control capacities



$$\frac{1}{C_G} = \frac{1}{C_Q} + \frac{1}{C_{ox}}$$



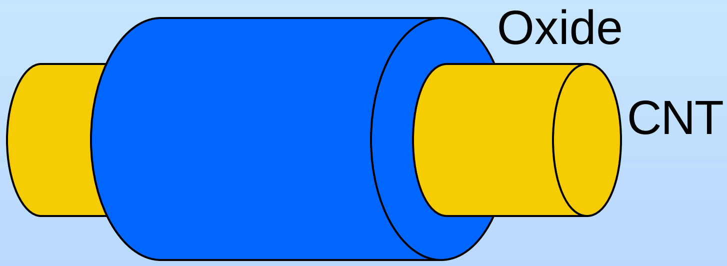
$$\frac{1}{C_Q} = \frac{1}{C_E} + \frac{1}{C_D}$$

$$C_D = e^2 D\left(E_f\right) \qquad C_E = \left(-\frac{\partial E_l}{\partial Q}\right)^{-1}$$

(S.Luryi, *Appl.Phys.Lett*. 52, 501 (1988), sistemi 2DES)

Gate capacitance

Gate is a Macroscopic metal



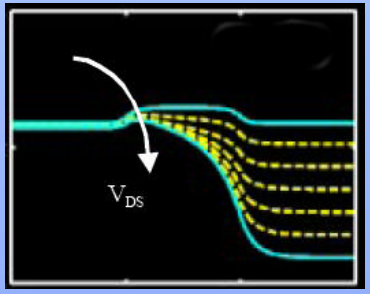
$$C_{ox} = \frac{2pke}{\ln(R_G / R_{CNT})}$$

In a classic MOS $C_Q >> C_{ox}$ => modulation depends on C_{ox}

In a well-tempered MOS $C_G >> C_S, C_D$

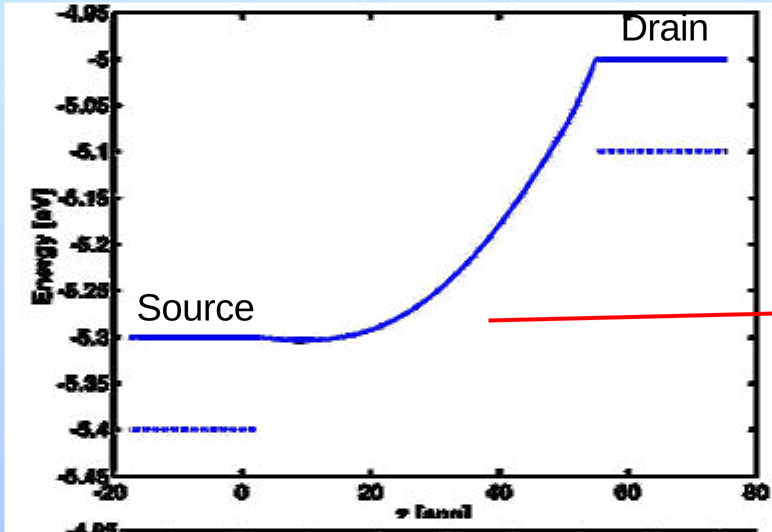
In 1D systems C_Q is small

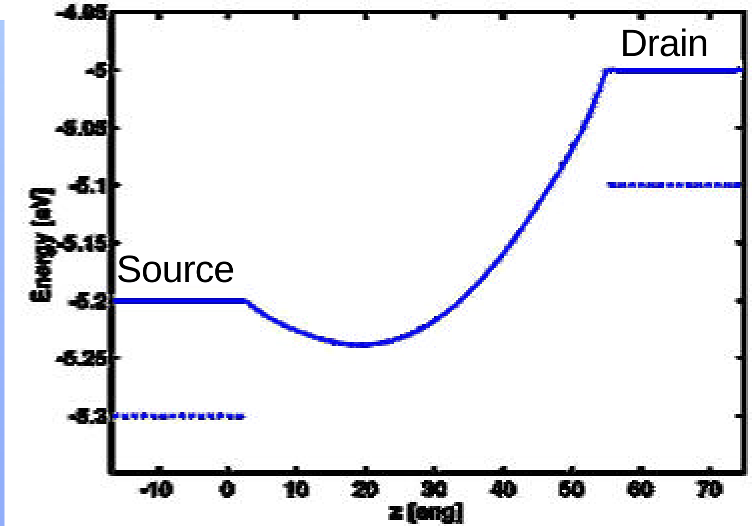
V_{ds} can influence the channel charge and barrier

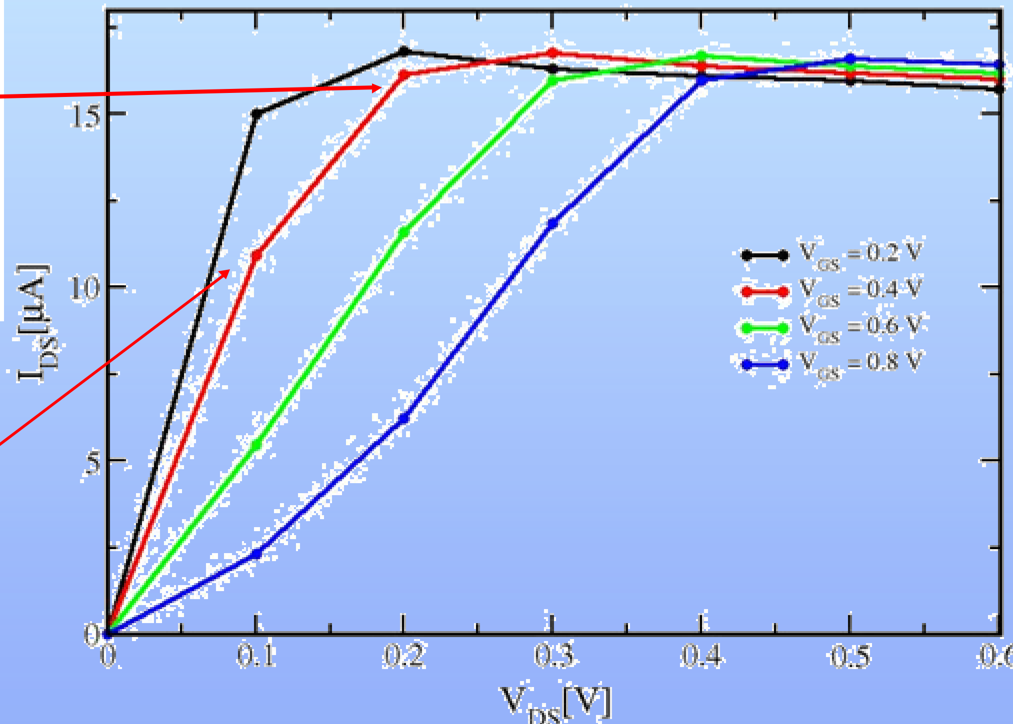


Caratteristiche di uscita I_{DS}/V_{DS}

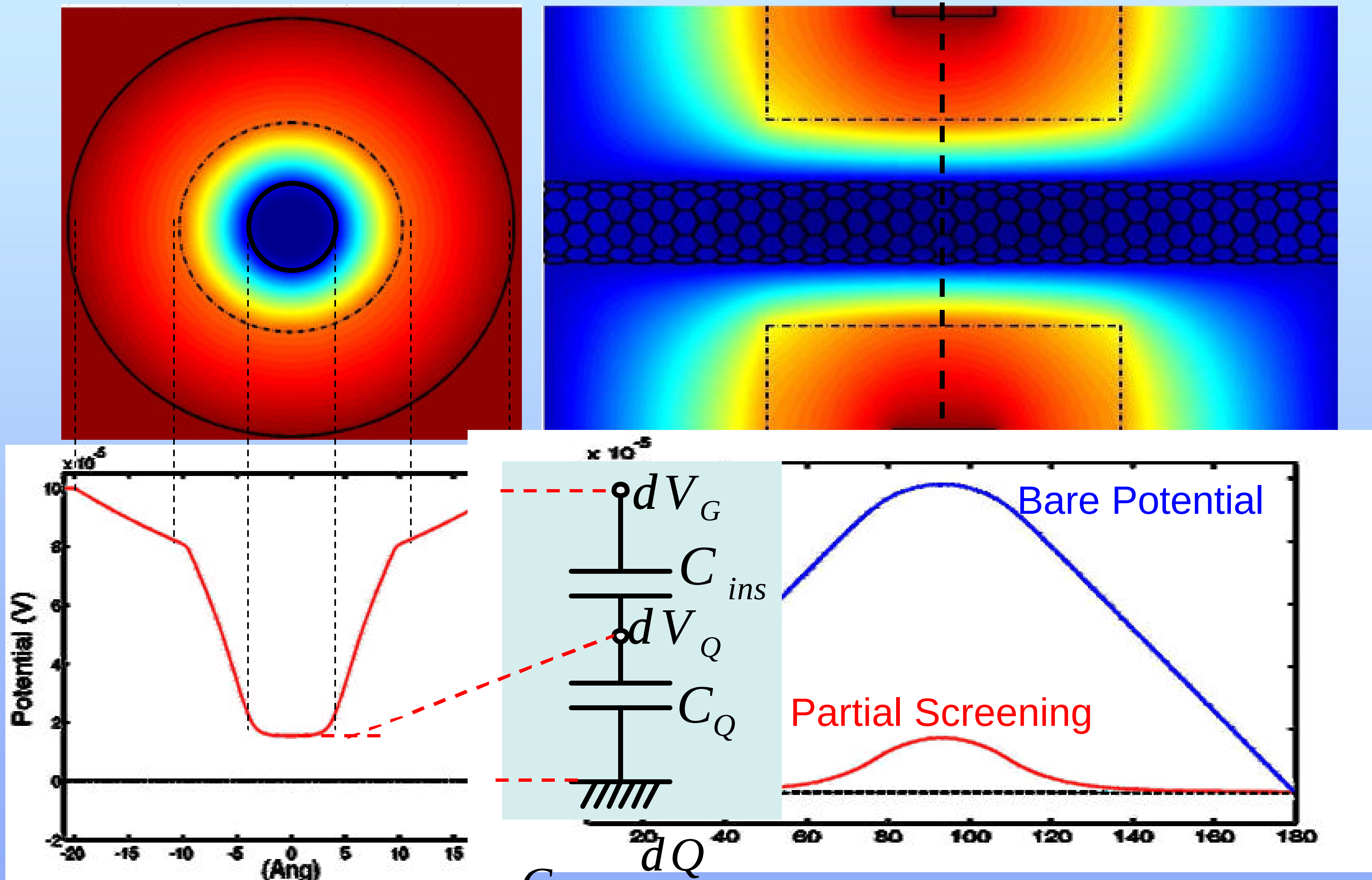
$$I = \frac{2e}{h}\int_{-\infty}^{+\infty} Tr\left[\Gamma_2 G^R \Gamma_1 G^A\right]\left(f_2 - f_1\right)dE$$





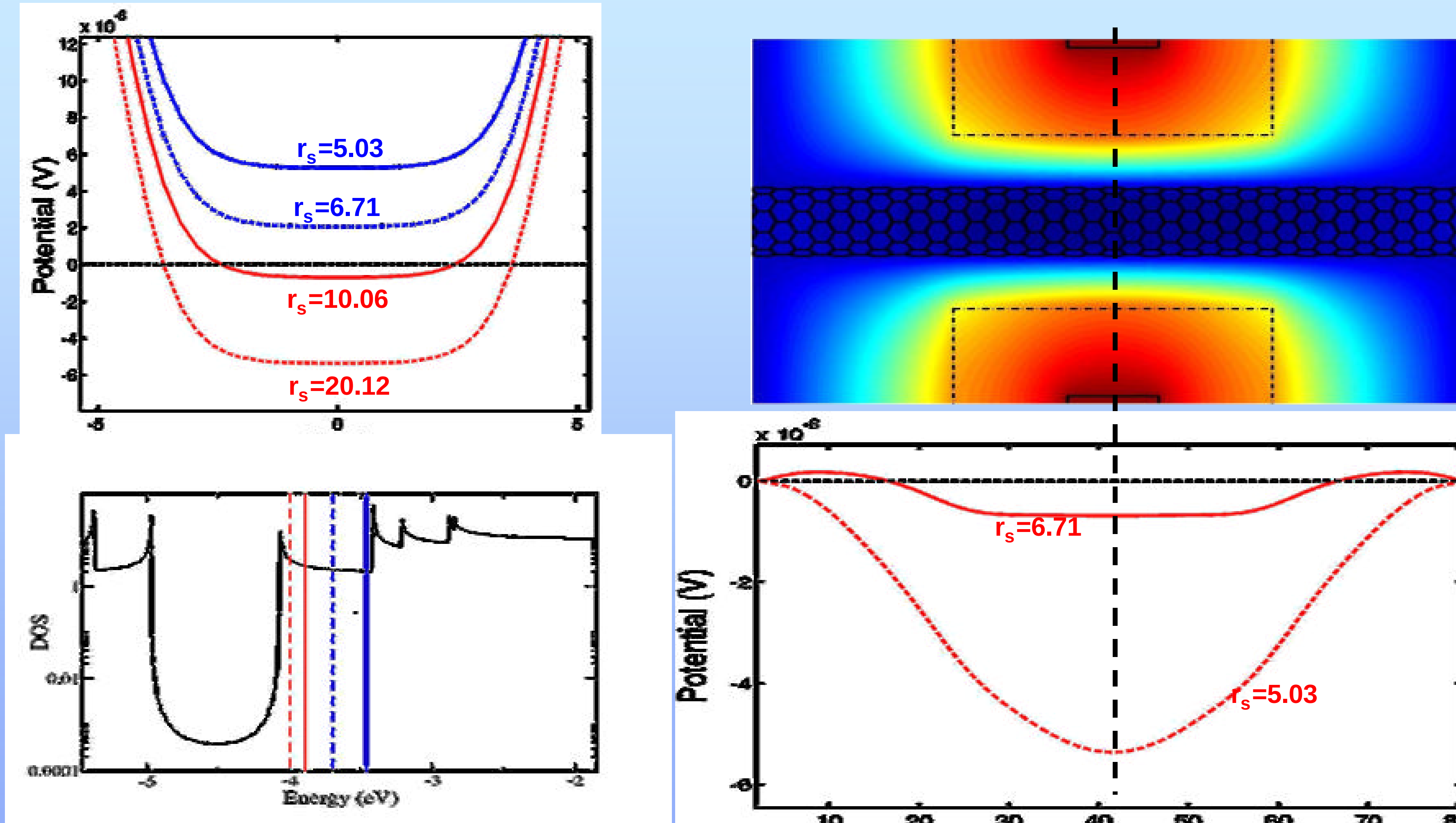


Calculation of C_Q



$$C_Q = \frac{dQ}{dV_Q}$$

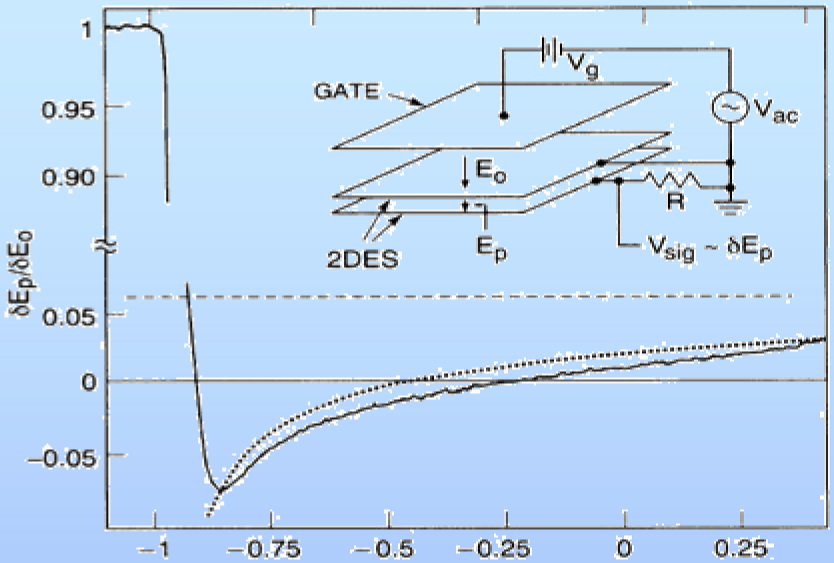
Over-screening in CNT



Negative C_Q ⟶ $C_{tot} > C_{ins}$

The can CNT better than a metal!

Negative compressibility



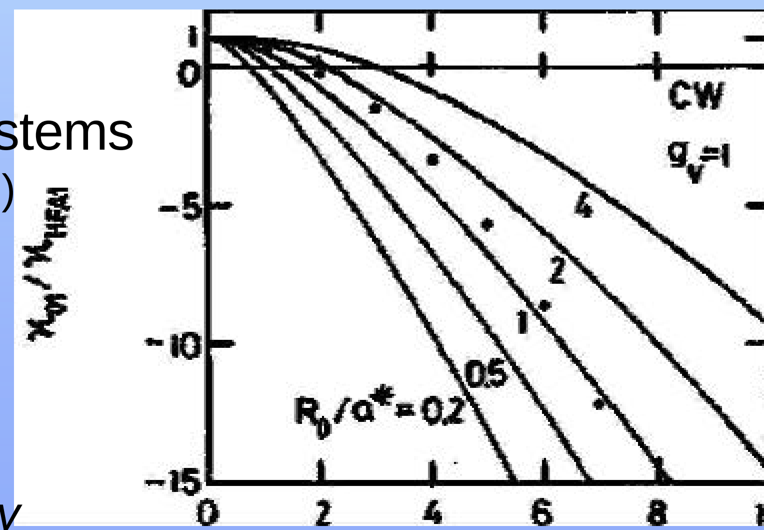
Experimental measurements in GaAs quantum wells

J.P.Eisenstein et al., *Phys.Rev.Lett*. 68, 647 (1992)

$$K^{-1} = n^2 \frac{\partial m}{\partial n} \quad \text{Ü Þ} \quad C_Q{}^{-1} = \frac{\partial m}{\partial Q}$$

Analytic results for quasi-1D electron systems

L.Calmels, A.Gold, *Phys. Rev.B*. 53, 10846 (1996)



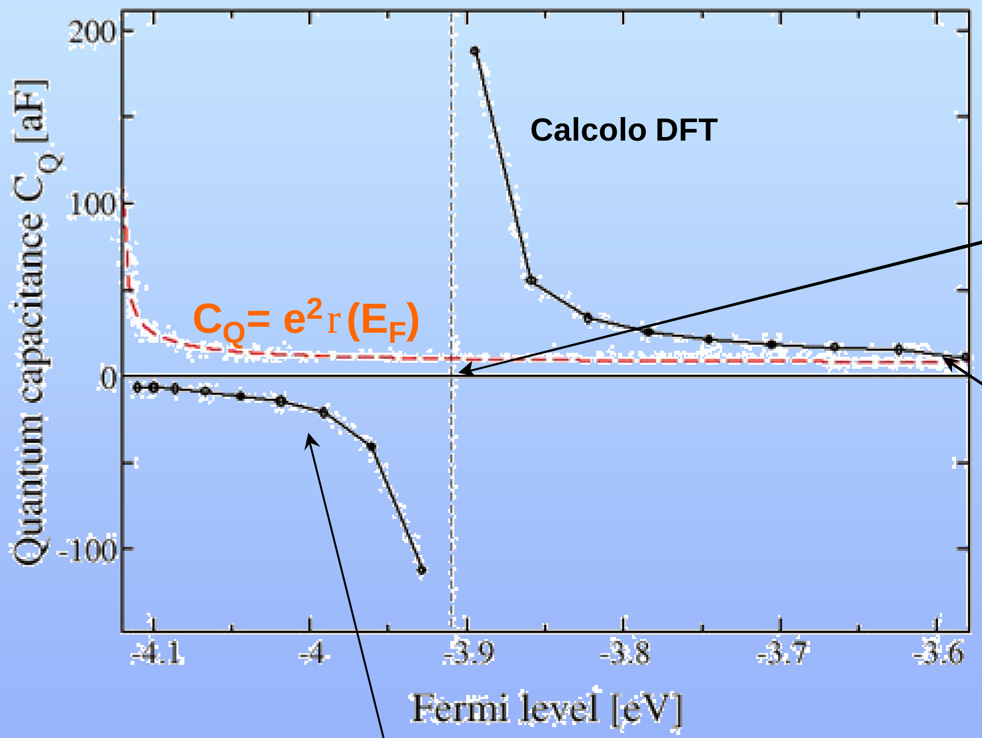
$$\frac{L_{CNT}}{C_Q} = \frac{1}{e^2 r\left(E_F\right)} \frac{K_0}{K_{HFA}}$$

K_0: free electrons compressibility

K_{HFA}: Hartree-Fock exchange compress.

Many-body exchange effect

$$C_Q = e^2 r\left(E_F\right)\frac{K_{XC}}{K_0}$$



Charge carrier density n_C:
TOTAL SCREENING
CNT ~ macroscopico

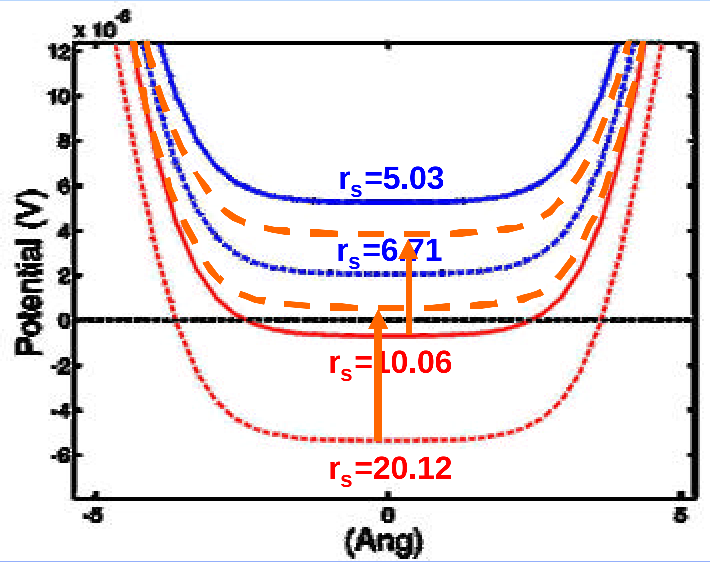
High density:
PARTIAL SCREENING
Dominated by DOS

Low density: *OVER-SCREENING*
Exchange interaction preveal

XC in *gDFTB*

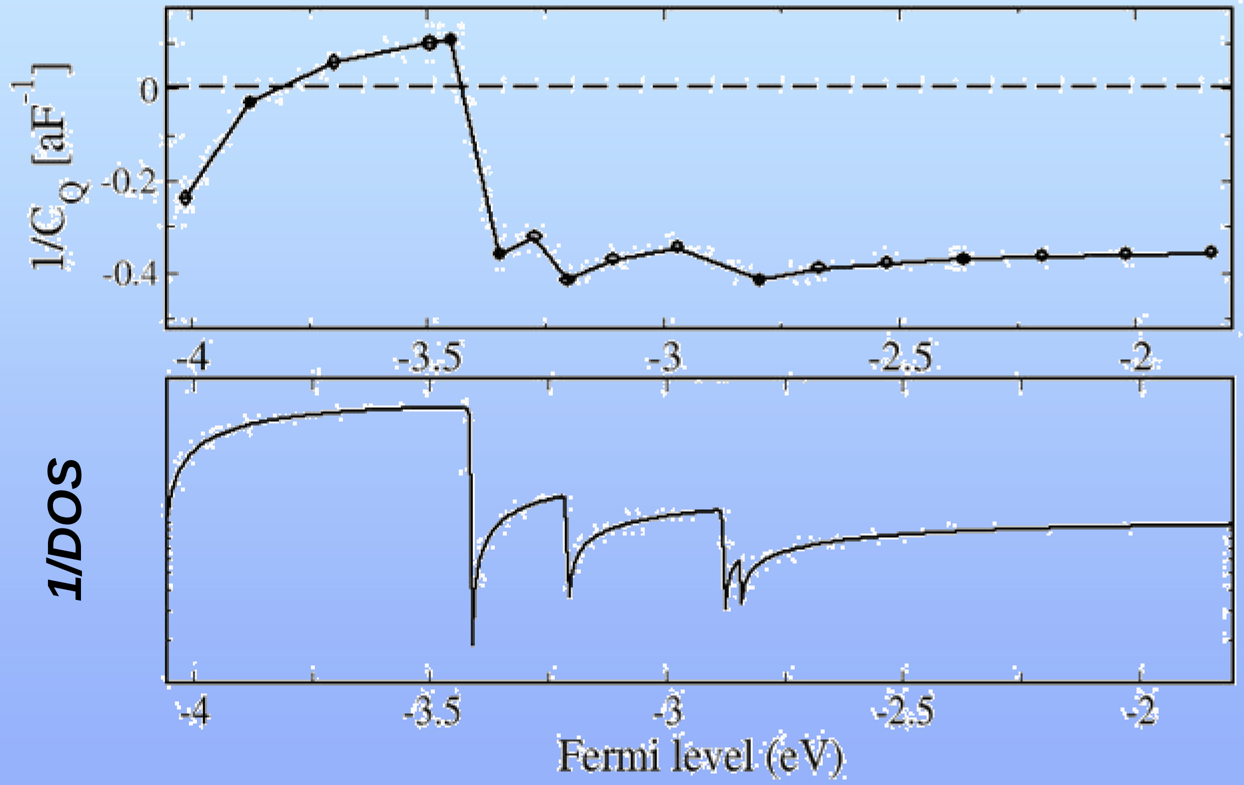
In DFTB the XC term is treated with a Hubbard on-site energy

Substituting U_H with U_{ee} accounts only for Hartree



The capacity becomes positive again

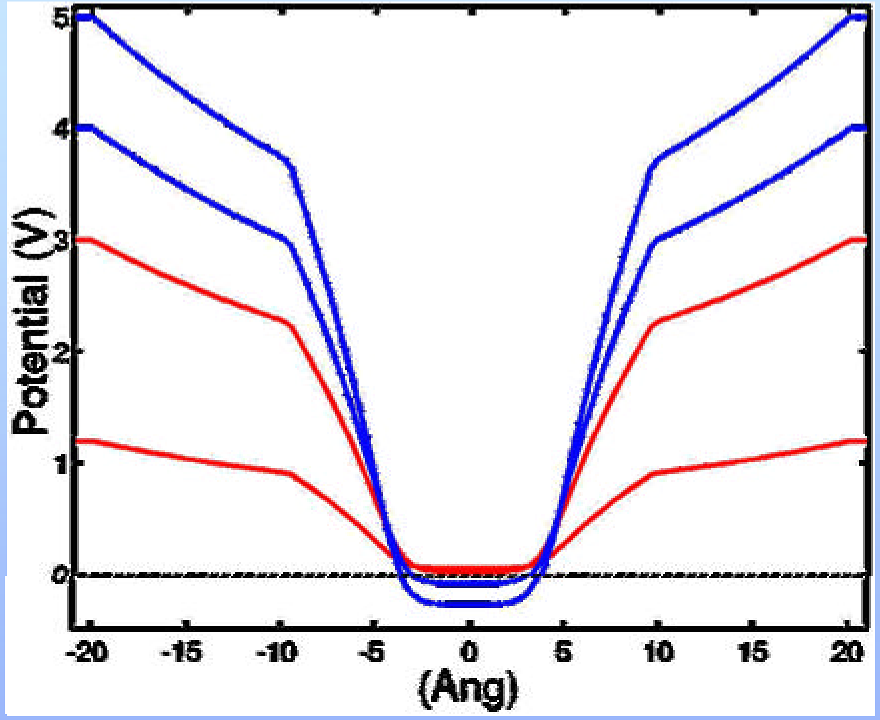
Quantum Capacitance vs DOS

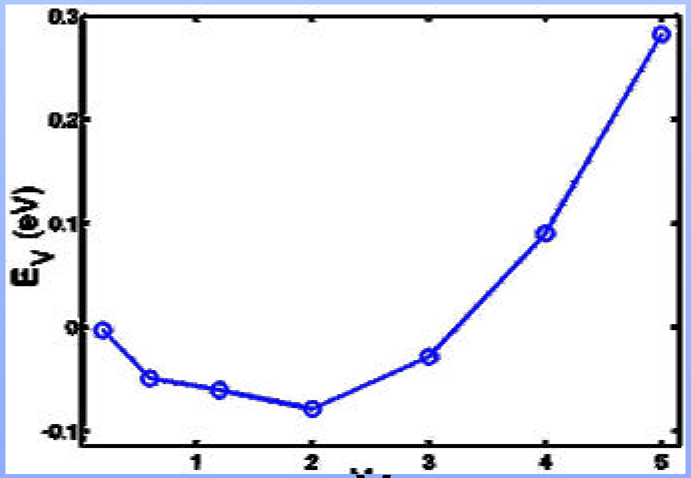


$$\frac{L_{CNT}}{C} = \frac{1}{e^2 r\left(E_F\right)} \frac{K_0}{K}$$

Over-screening and modulation

V_{GS}





V_{GS}

Unconventional Trans-characteristics
Possible applications ?

Conclusions

Comprehensive calculation of Quantum Capacity in a CNT(10,0) using NEGF

XC effects can give deviations from “classical” C_Q

Negative C_Q below a crytical carrier density which compares well with analytic results in quasi 1D systems

More complicated behaviour when more subbands are occupied