Journal club preprint presentation

Contact dependence of carrier injection in carbon nanotubes: An *ab initio* study

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We combine *ab initio* density functional theory with transport calculations to provide a microscopic basis for distinguishing between 'good' and 'poor' metal contacts to nanotubes. Comparing Ti and Pd as examples of different contact metals, we trace back the observed superiority of Pd to the nature of the metal-nanotube hybridization. Based on large scale Landauer transport calculations, we suggest that the 'optimum' metal-nanotube contact combines a weak hybridization with a large contact length between the metal and the nanotube.

PACS numbers: 73.23.Ad, 73.40.Cg,73.63.Fg,73.63.Rt

(submitted)

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by Norbert Nemec

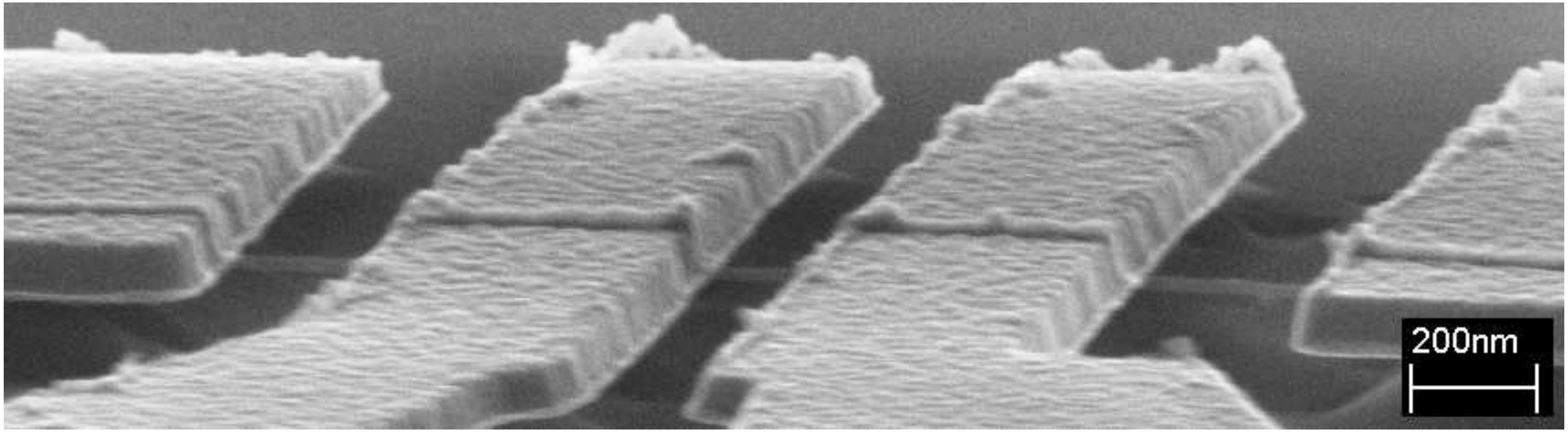
Outline

- motivation: contacting carbon nanotubes (CNTs)
- microscopic *ab-initio study* of the metal/CNT-interface
- extracting parameters for tight-binding (TB) calculations
- *TB-model* for large scale transport calculations
- evaluation of the contact resistance

- *work in progress:* non-epitaxial contacts

Motivation

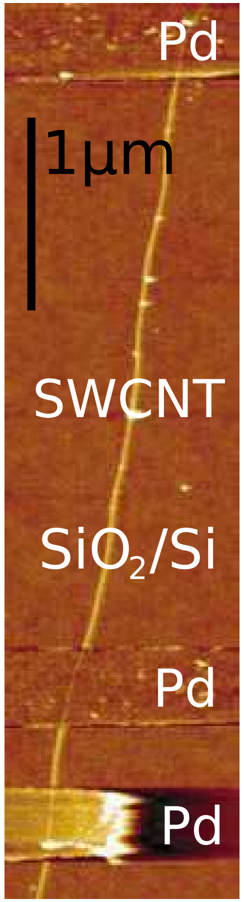
CNT-transport measurements – typical experimental setup:



(courtesy of C. Strunk, 2004 Regensburg)

- CNT on an insulating (underetched) substrate
- backgate control possible
- contacts $\gtrsim$100nm by metal evaporation (e.g. Au, Cr, Pd etc.)

Experimental facts and puzzles



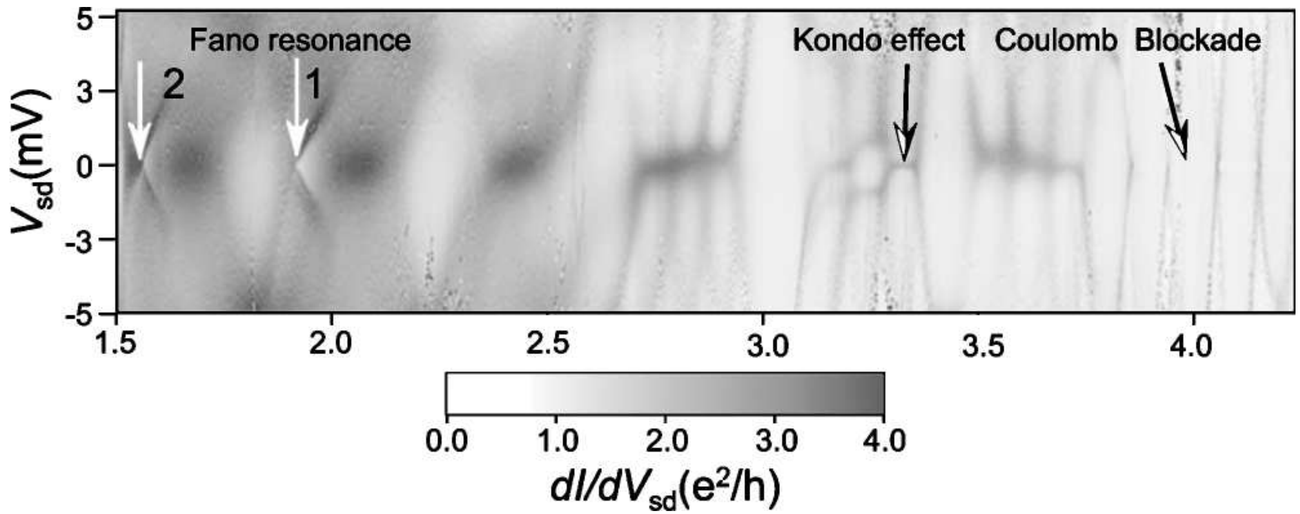
*Javey et al. Nature **424**, 654 (2003)*

- material dependent contact resistance:

$$\mathrm{Au/Cr} < \mathrm{Ti} < \mathrm{Pd}$$

- varying results about the *effective contact size*

- gate dependent contact resistance:

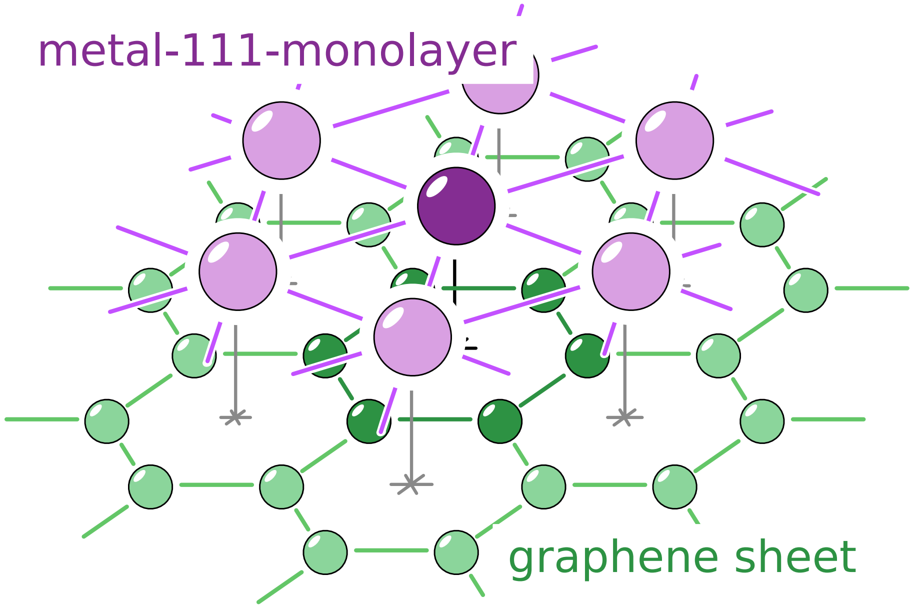


Babić *et al.* Phys. Rev. B **70**, 195408 (2004)

Electronic structure at the interface

***microscopic DFT-study, using SIESTA** (LDA-PZ)*

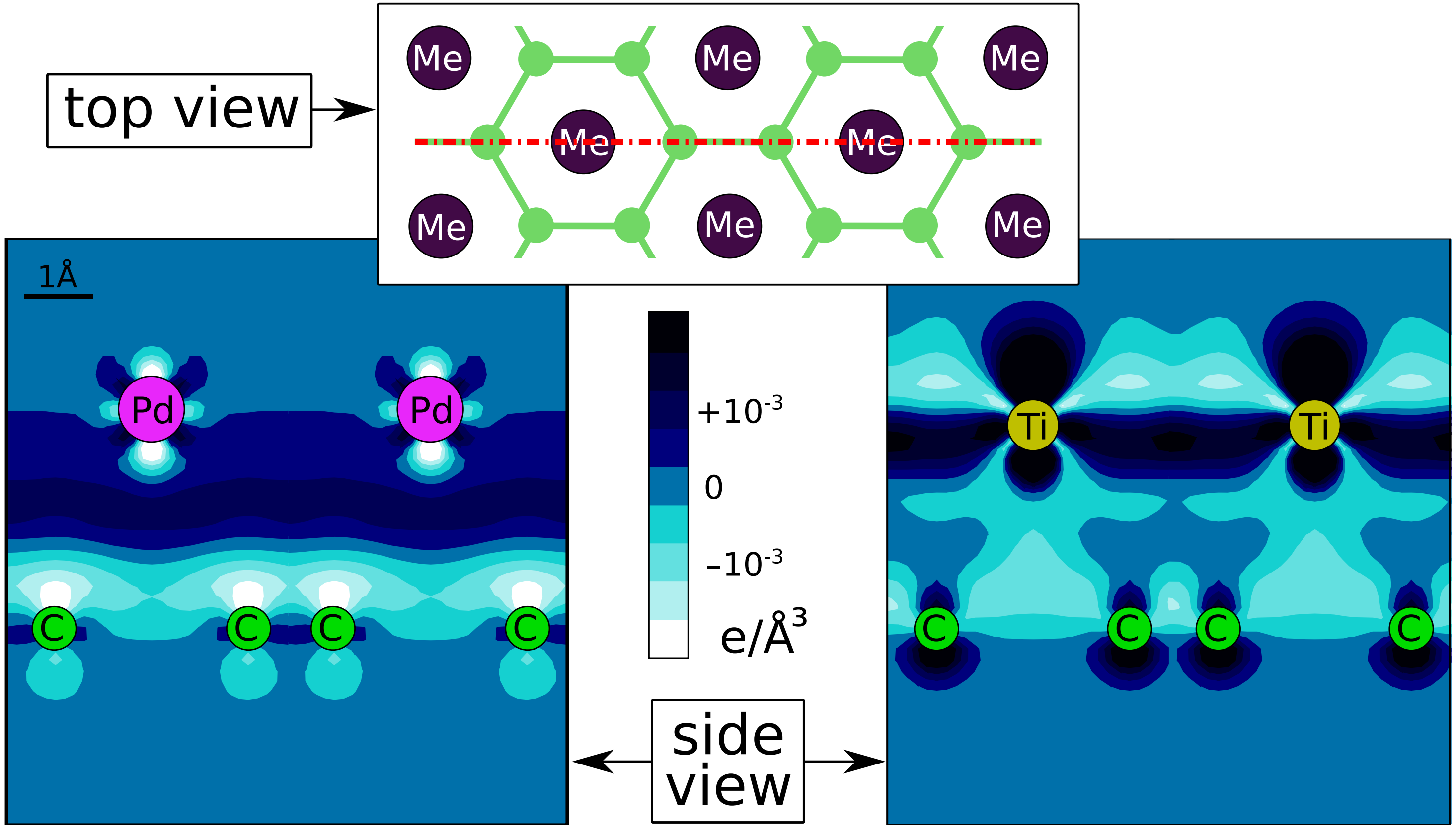
- metal/CNT interface modelled by graphene/metal-monolayer:



- lattice constant: 2.5 Å
- interlayer distance: 3.2 Å (Pd) 3.0 Å (Ti)
- alignment: sixfold hollow

Electron density redistribution

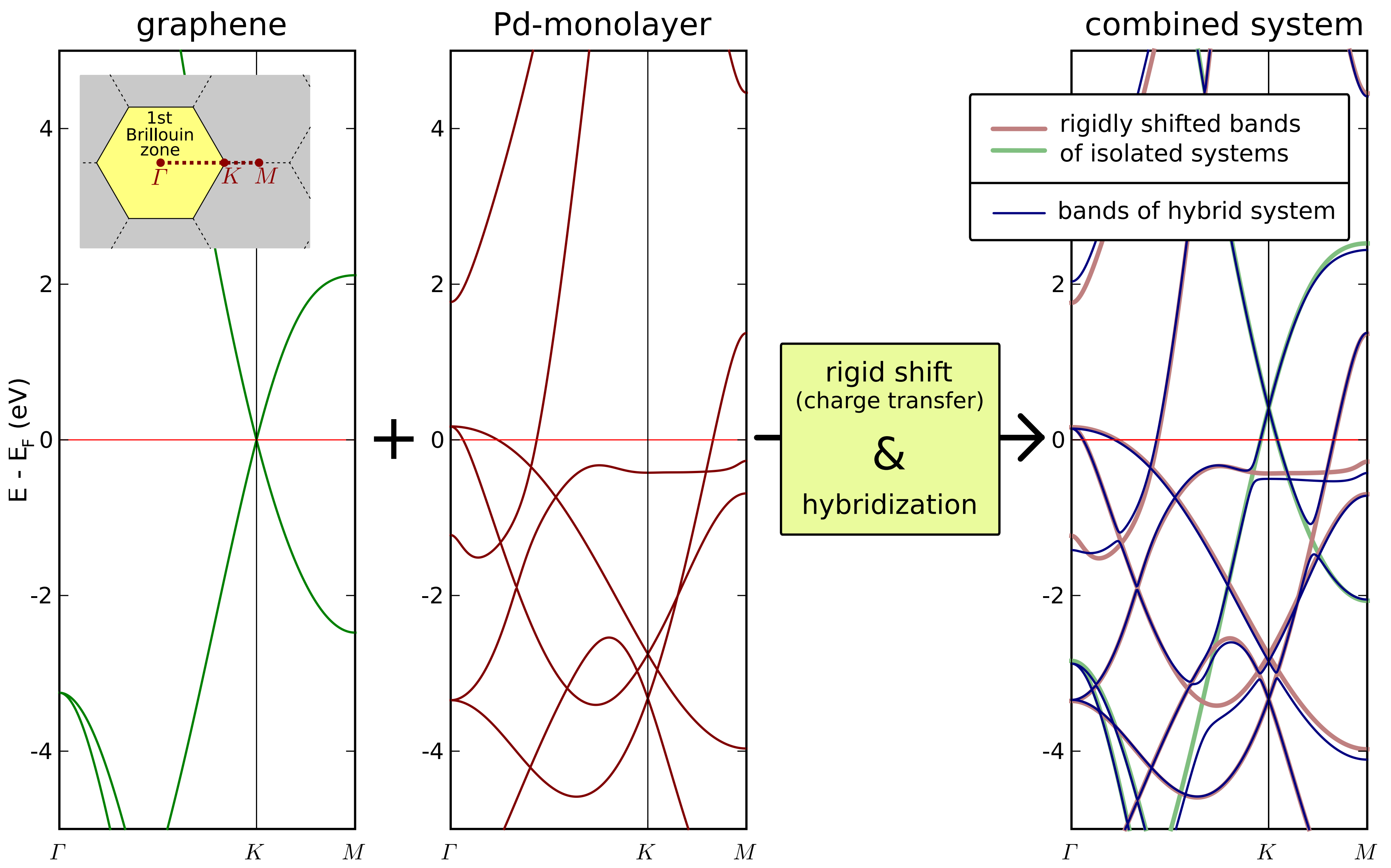
$$\Delta\rho(\boldsymbol{r}) \;:=\; \rho_{\mathrm{Me}/C}(\boldsymbol{r}) - \left(\rho_{\mathrm{Me}}(\boldsymbol{r}) + \rho_C(\boldsymbol{r})\right)$$



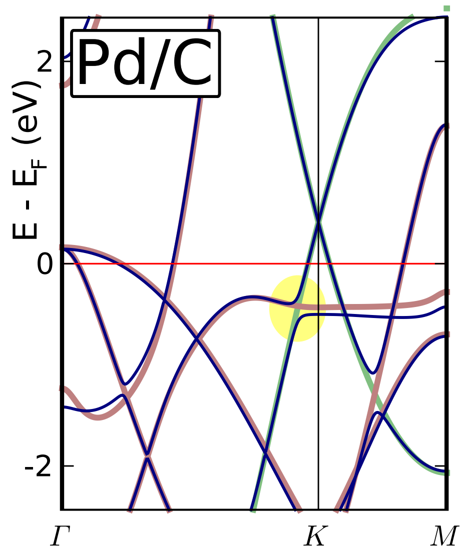
Pd: accumulation of electrons in interlayer region

$\Rightarrow$ lowering of the scattering potential at the interface?

Band structure of hybrid system



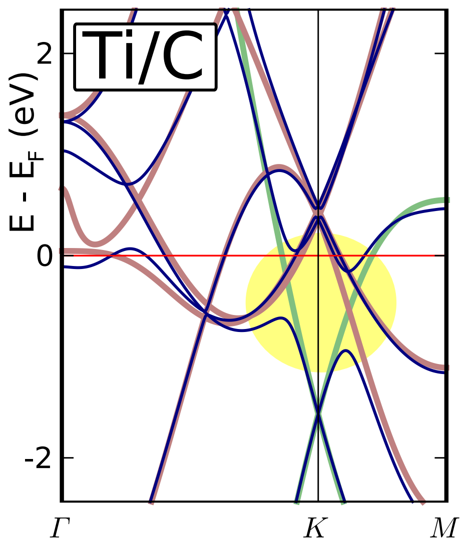
Band structure at contact: Ti vs. Pd



electron-transfer: *from graphene to Pd*

rigid shift of graphene bands: $\Delta E = 0.41\,\mathrm{eV}$

weak hybridization near K-point: $\sim 0.15\,\mathrm{eV}$



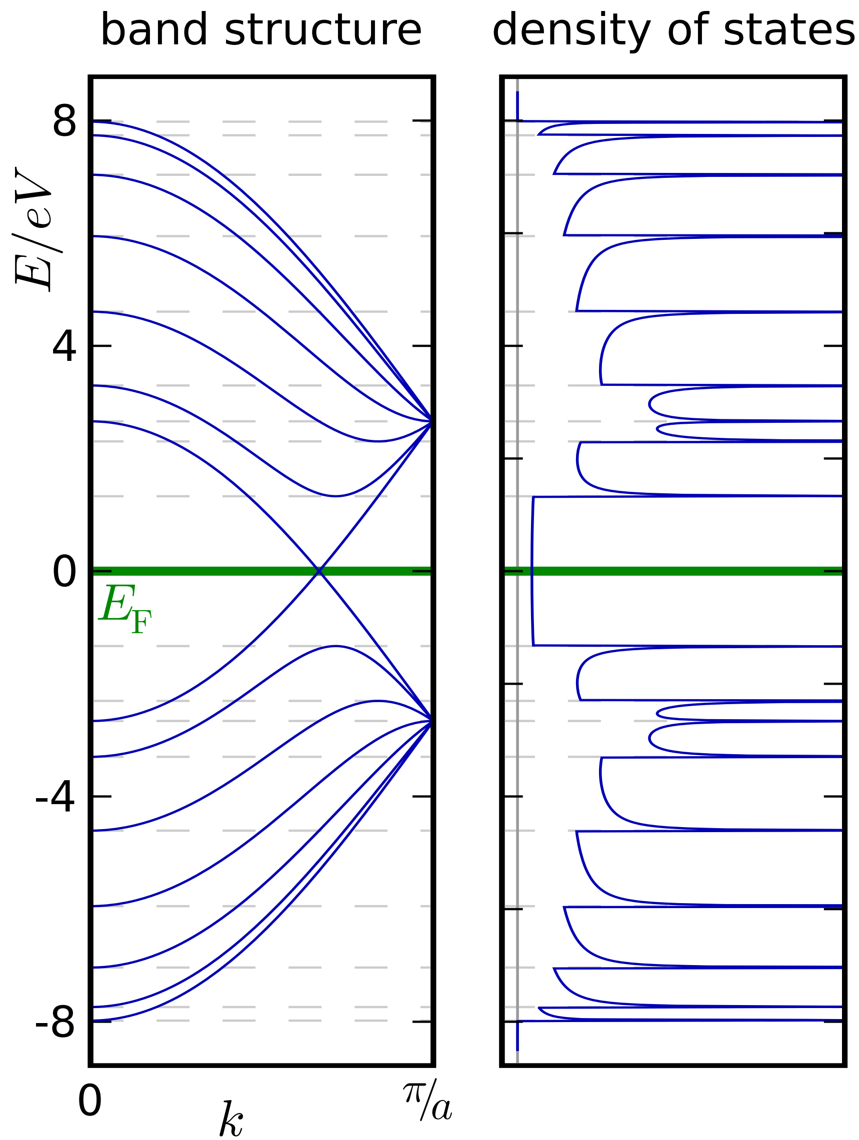
electron-transfer: *from Ti to graphene*

rigid shift of graphene bands: $\Delta E = -1.56\,\mathrm{eV}$

strong hybridization near K-point: $\sim 0.80\,\mathrm{eV}$

CNTs in TB-approximation

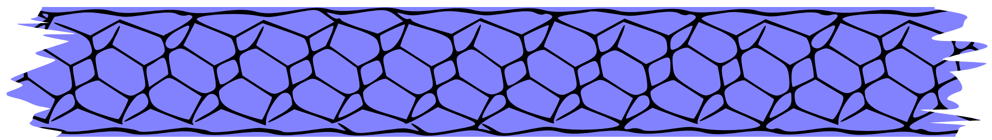
CNT (6,6)



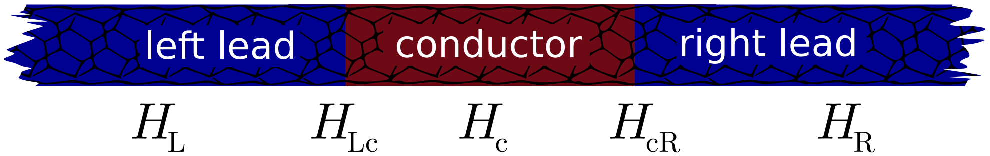
Hamiltonian:

(π-orbital tight-binding)

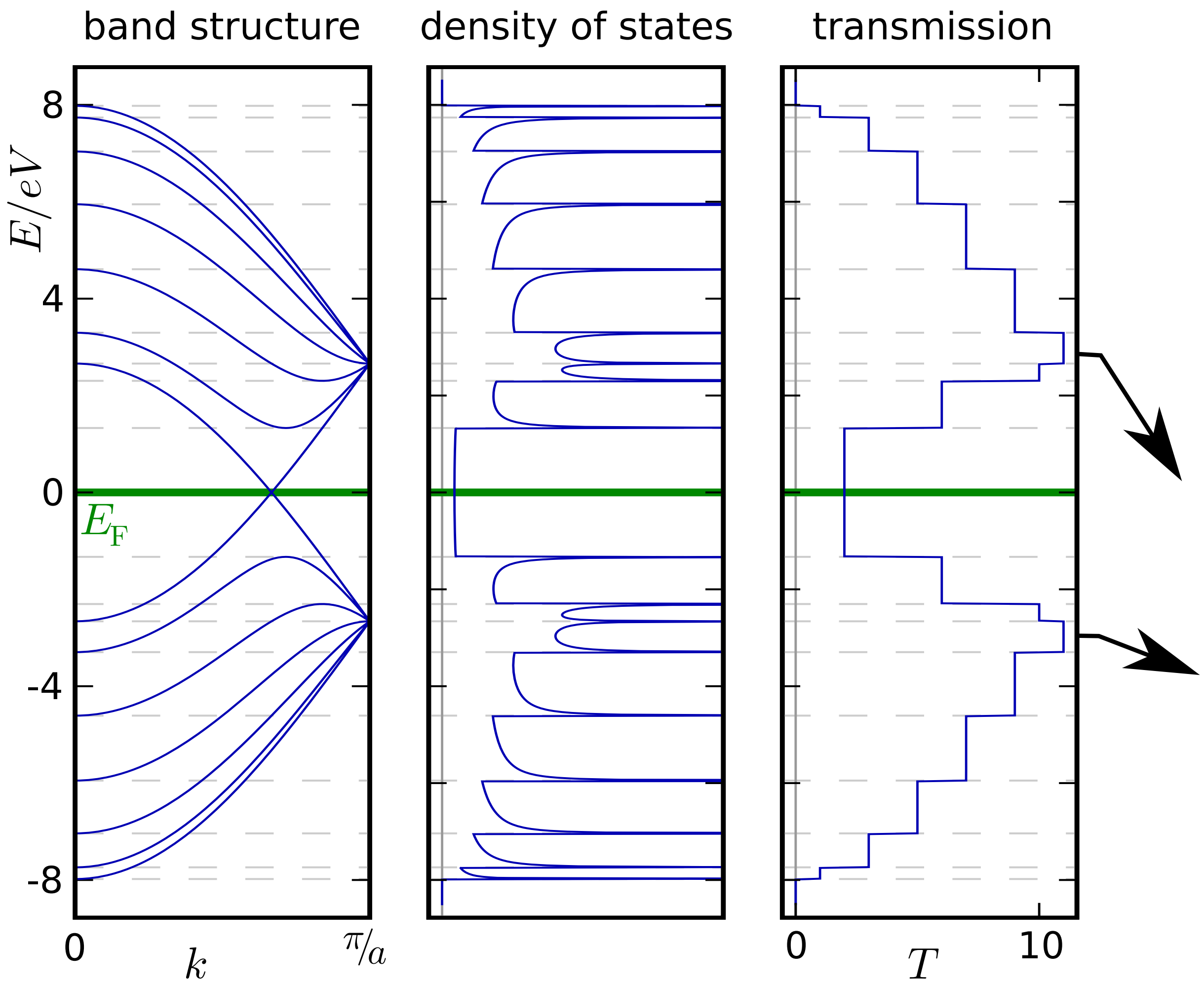
$$H = \sum_i \varepsilon_0 \, c_i^\dagger c_i + \sum_{\langle i,j \rangle} \gamma_{ij} \, c_i^\dagger c_j$$



Landauer transport



CNT (6,6)



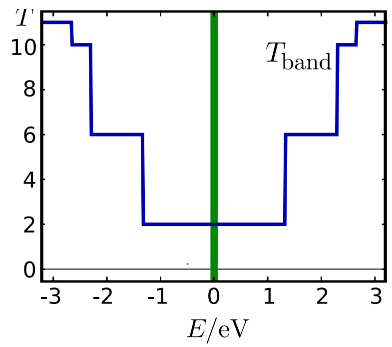
Landauer conductance:

$$G = \frac{2e^2}{h} T(E_F)$$

where $T = \sum_{n=1}^{N_{\mathrm{ch}}} T_n$

Fisher-Lee relation:

$$T = \mathrm{tr}\, \Gamma_{\mathrm{L}} G^{\mathrm{r}} \Gamma_{\mathrm{R}} G^{\mathrm{a}}$$

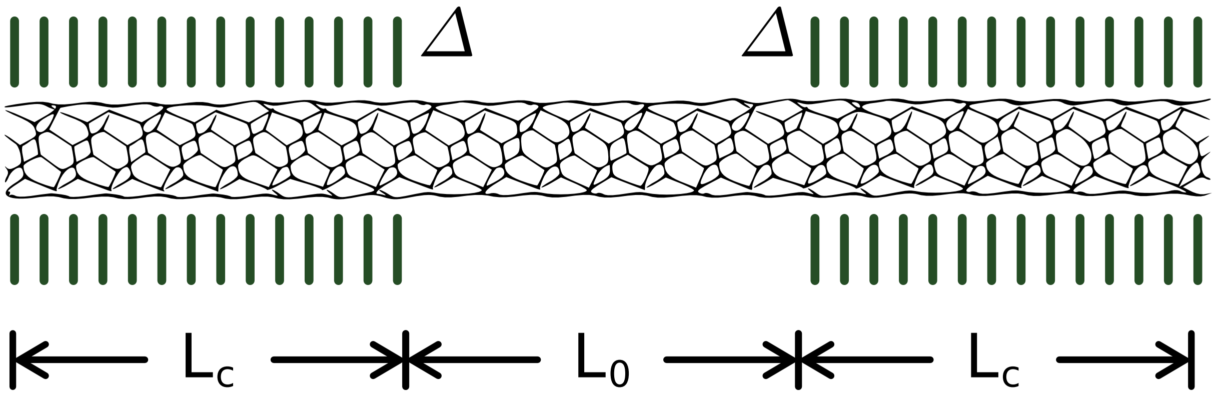


Coating wide-band leads

wide-band approximation:

$$\Sigma = -\mathrm{i}\Delta$$

(independent for each atom, independent of energy)



$L_0 = 100\,\mathrm{nm}$ (fixed), $L_c \leqslant 100\,\mathrm{nm}$ (variable)

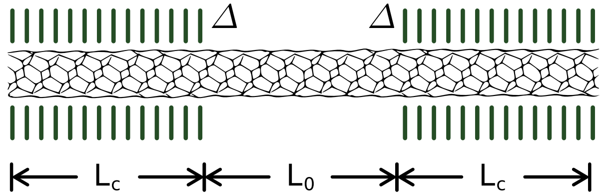
Wide-band constant Δ

$$\Delta = \left(\gamma_{\text{carbon metal}}\right)^2 \times \mathrm{LDOS}_{\text{metal-surface}}$$

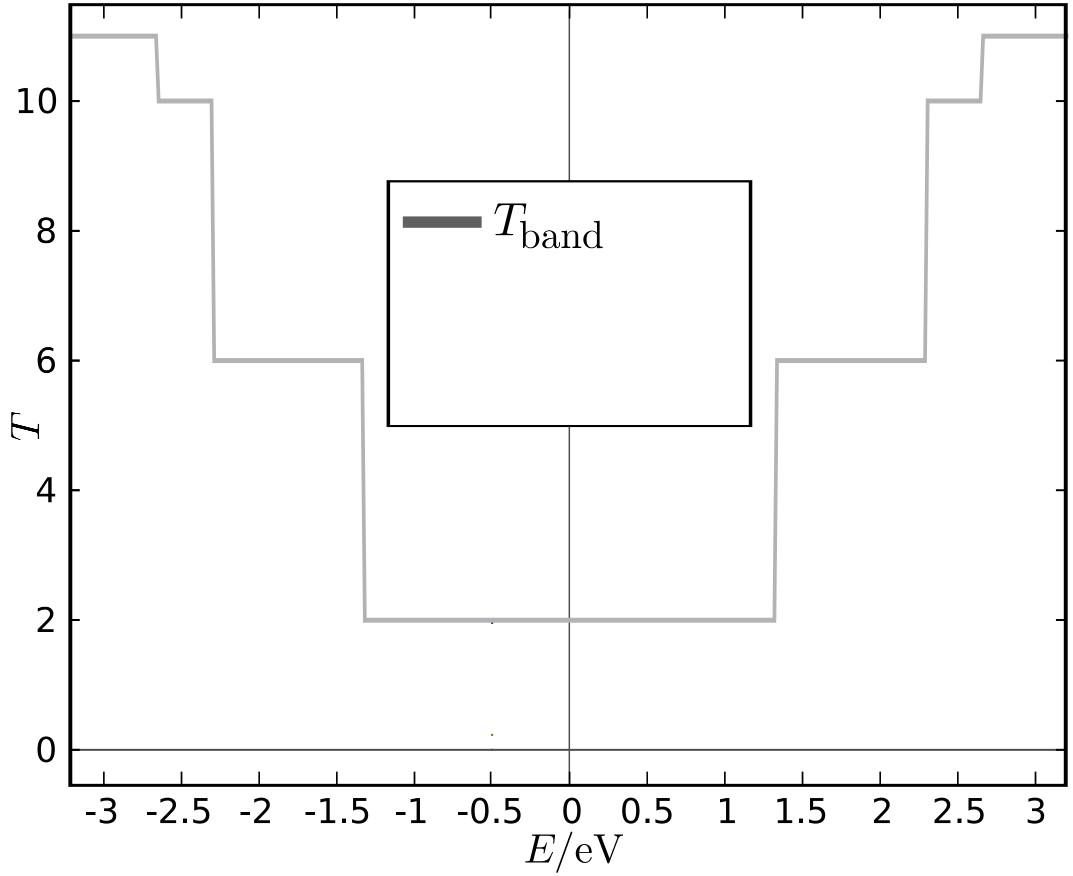
From ab initio calculation:

$\Delta_{\mathrm{Pd}} \approx 0.02\,\mathrm{eV}$, $\Delta_{\mathrm{Ti}} \approx 0.10\,\mathrm{eV}$

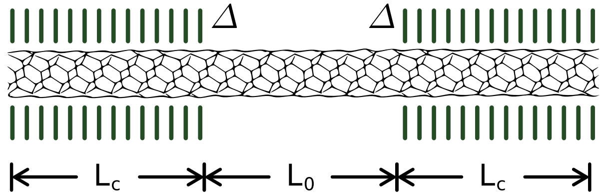
Transmission with coating wide-band leads



Raw transmission data $T_\Delta(E)$ and $T_{\mathrm{band}}(E)$:



Transmission with coating wide-band leads



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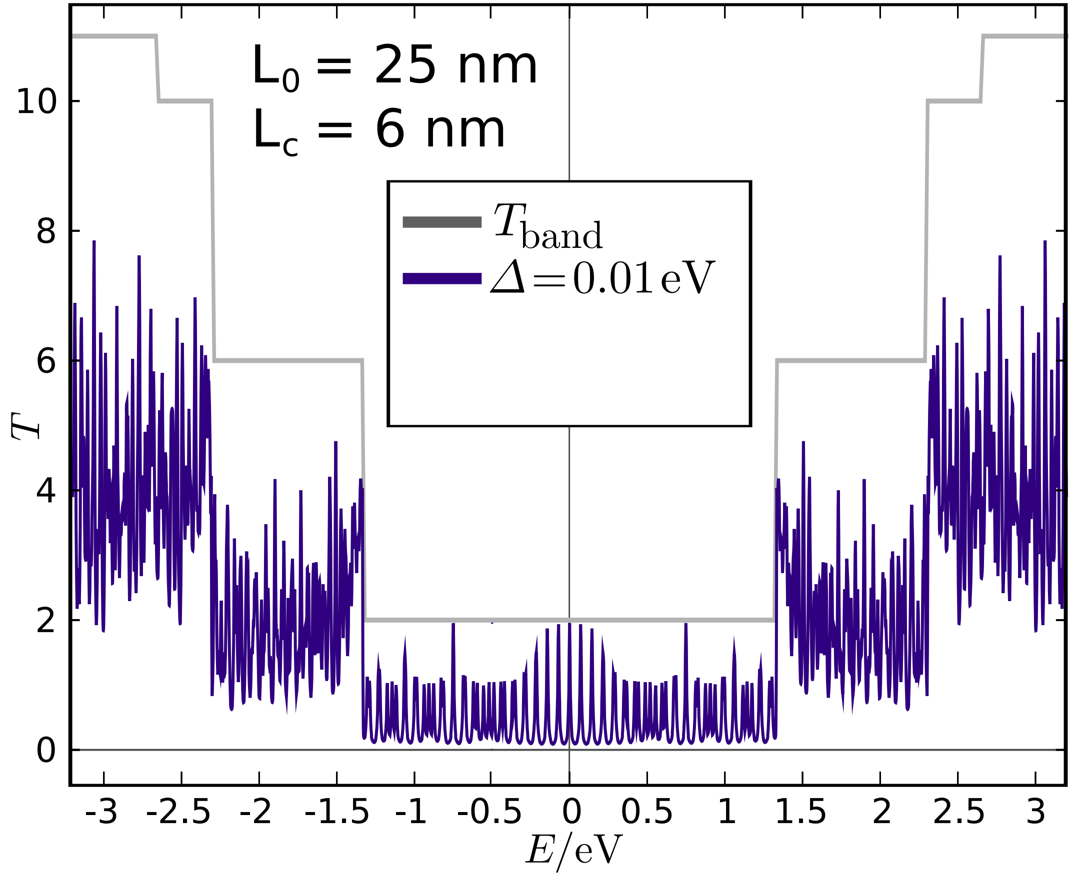
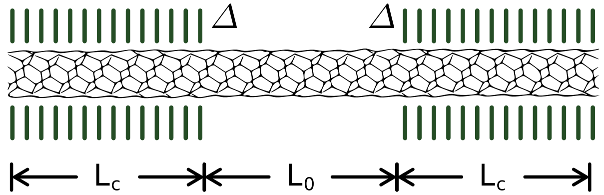


For fixed length L_c:

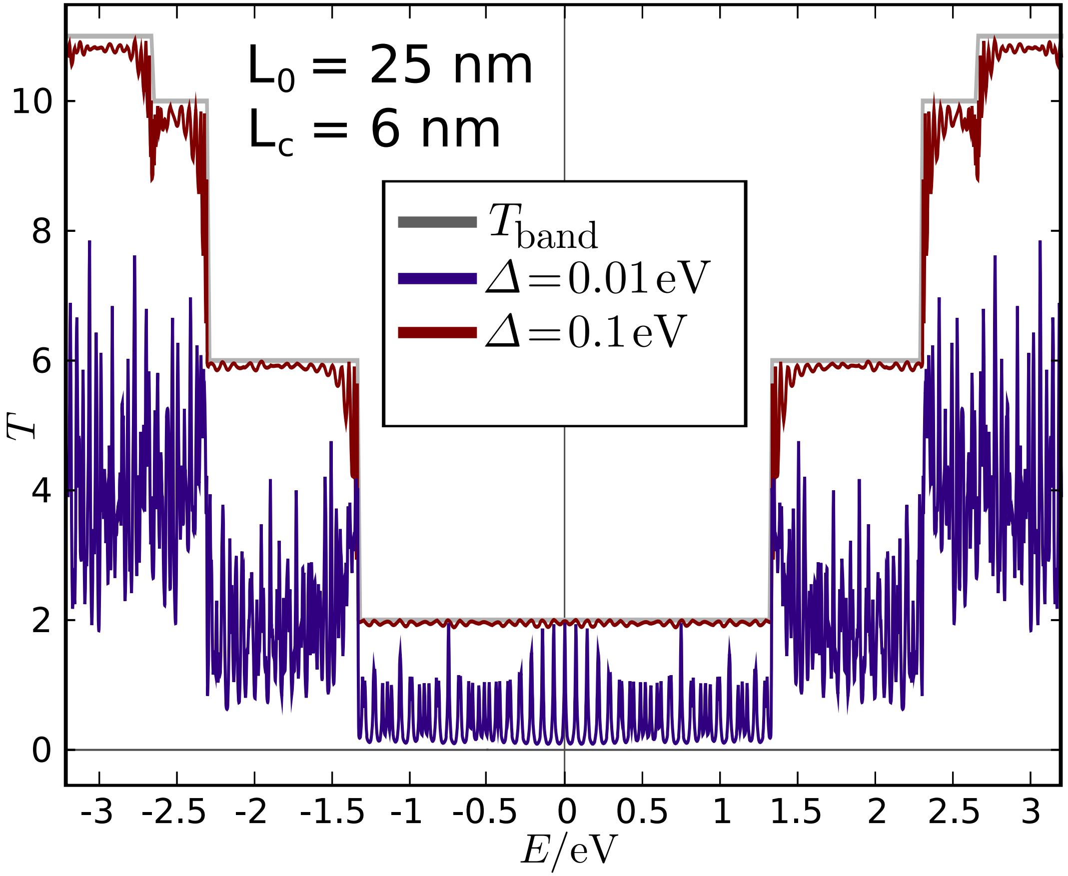
weak coupling Δ:

resonant tunneling (whole tube)

Transmission with coating wide-band leads



Raw transmission data $T_\Delta(E)$ and $T_{\text{band}}(E)$:

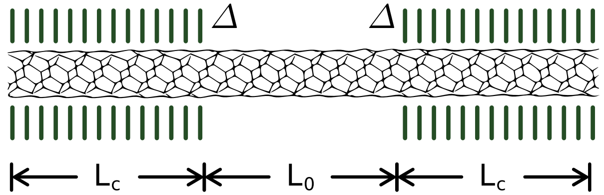


For fixed length L_c:

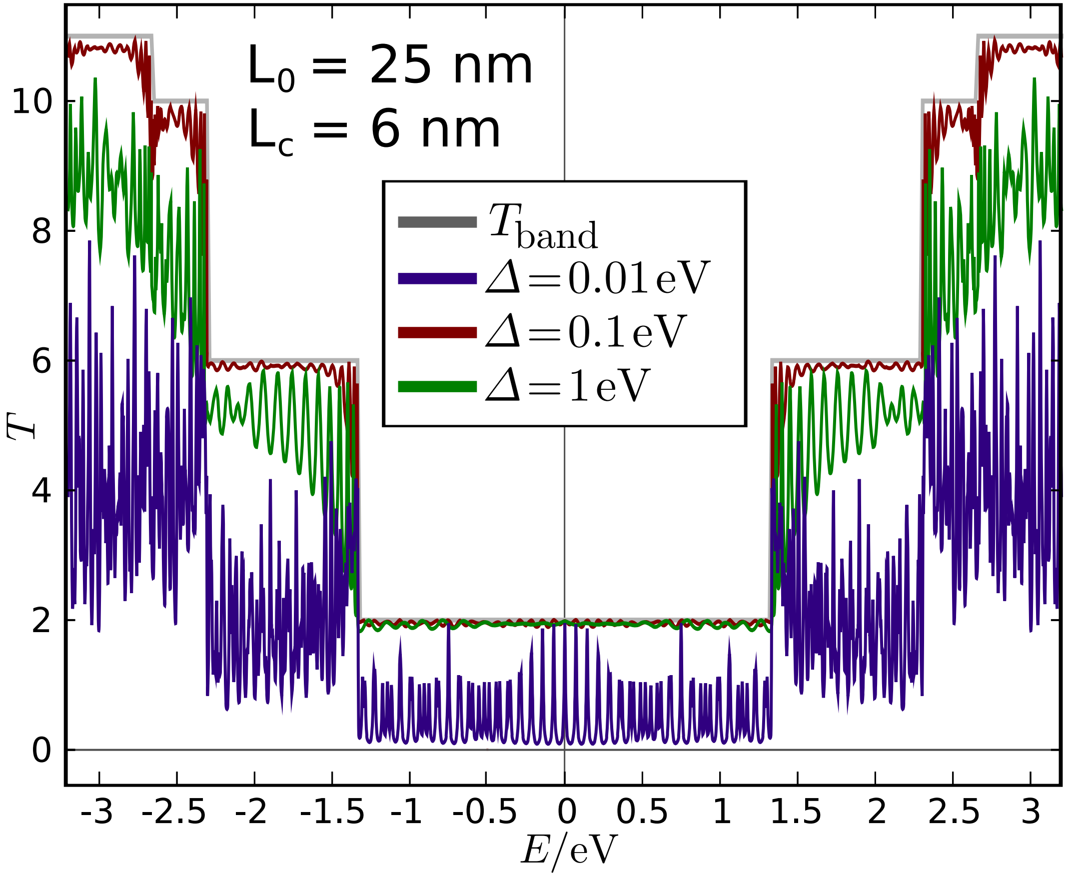
weak coupling Δ:
resonant tunneling (whole tube)

intermediate coupling Δ:
nearly perfect transmission

Transmission with coating wide-band leads



Raw transmission data $T_\Delta(E)$ and $T_{\text{band}}(E)$:



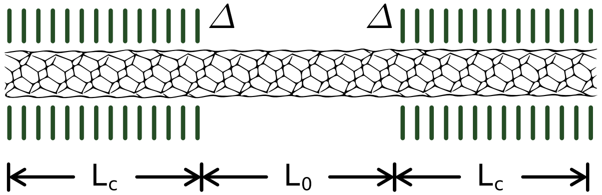
For fixed length L_c:

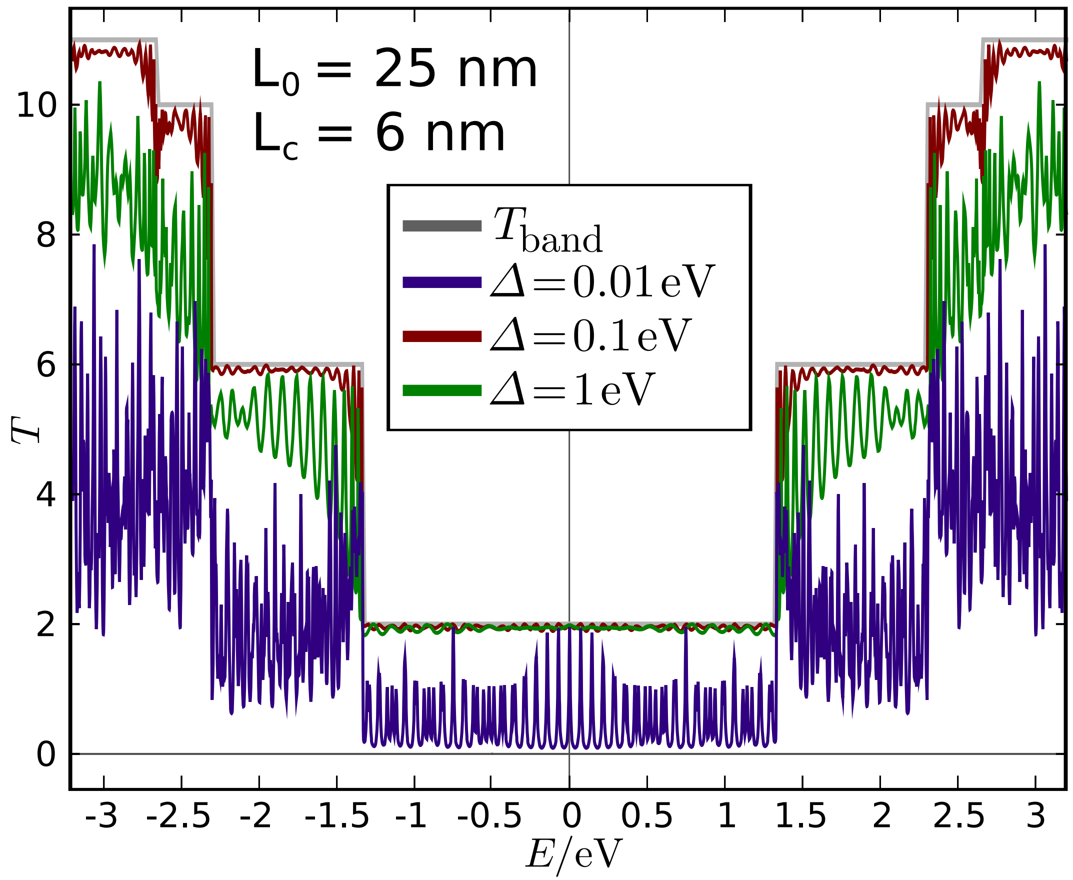
weak coupling Δ:
resonant tunneling (whole tube)

intermediate coupling Δ:
nearly perfect transmission

strong coupling Δ:
resonant tunneling (central region)

Contact resistance

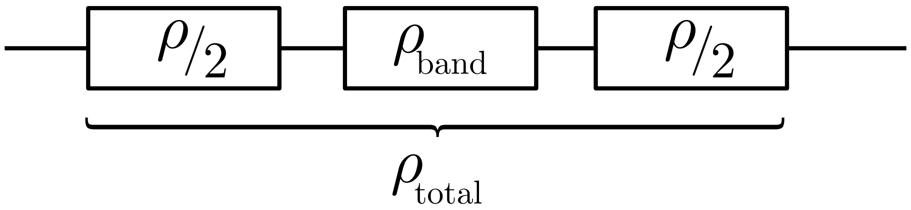




$$\tau_\Delta := \langle T_\Delta \rangle_E$$

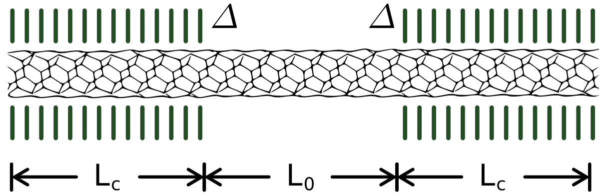
(cover several resonances, massless bands only)

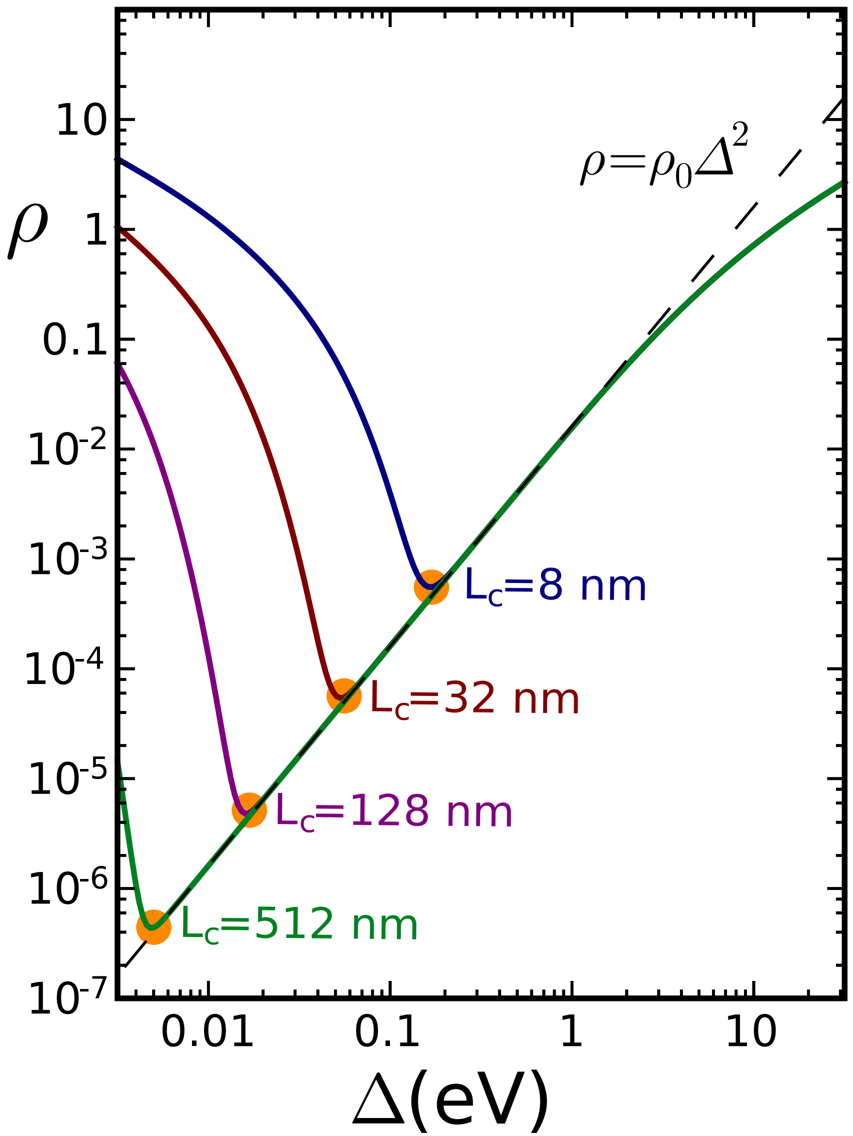
$$\rho_{\text{total}} := 1/\tau_\Delta$$
$$\rho_{\text{band}} := 1/T_{\text{band}}$$



$$\rho \ := \ \rho_{\text{total}} - \rho_{\text{band}}$$

Results for fixed L_c





Optimum transmission at $\Delta_{\mathrm{opt}}(L_c)$

$\Delta < \Delta_{\mathrm{opt}}$: *weak coupling* regime

$\rightarrow$ conventional Breit-Wigner broadening of individual resonances

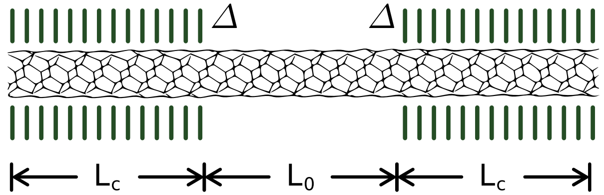
$\Delta > \Delta_{\mathrm{opt}}$: *strong coupling* regime

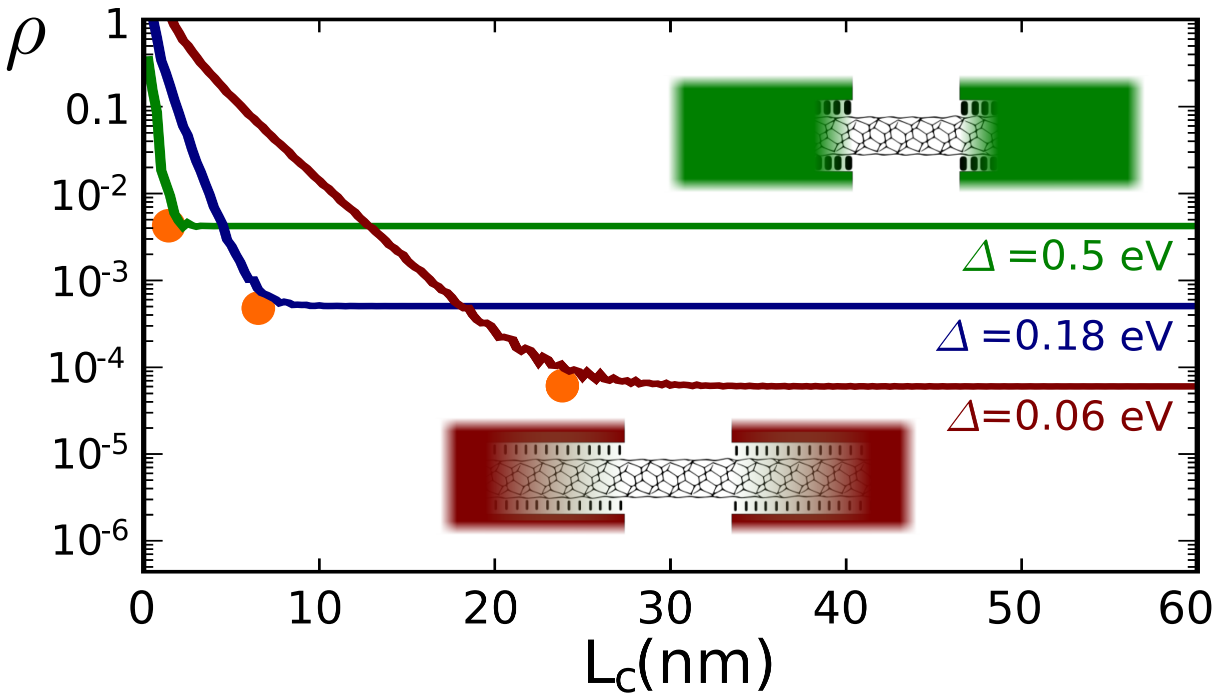
L_c has no effect

(CNT effectively *cut off* at contact-edge)

$\rightarrow$ inverse Breit-Wigner broadening of individual resonances

Results for fixed Δ

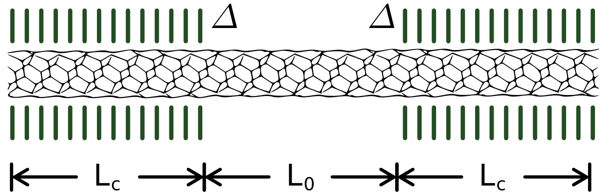


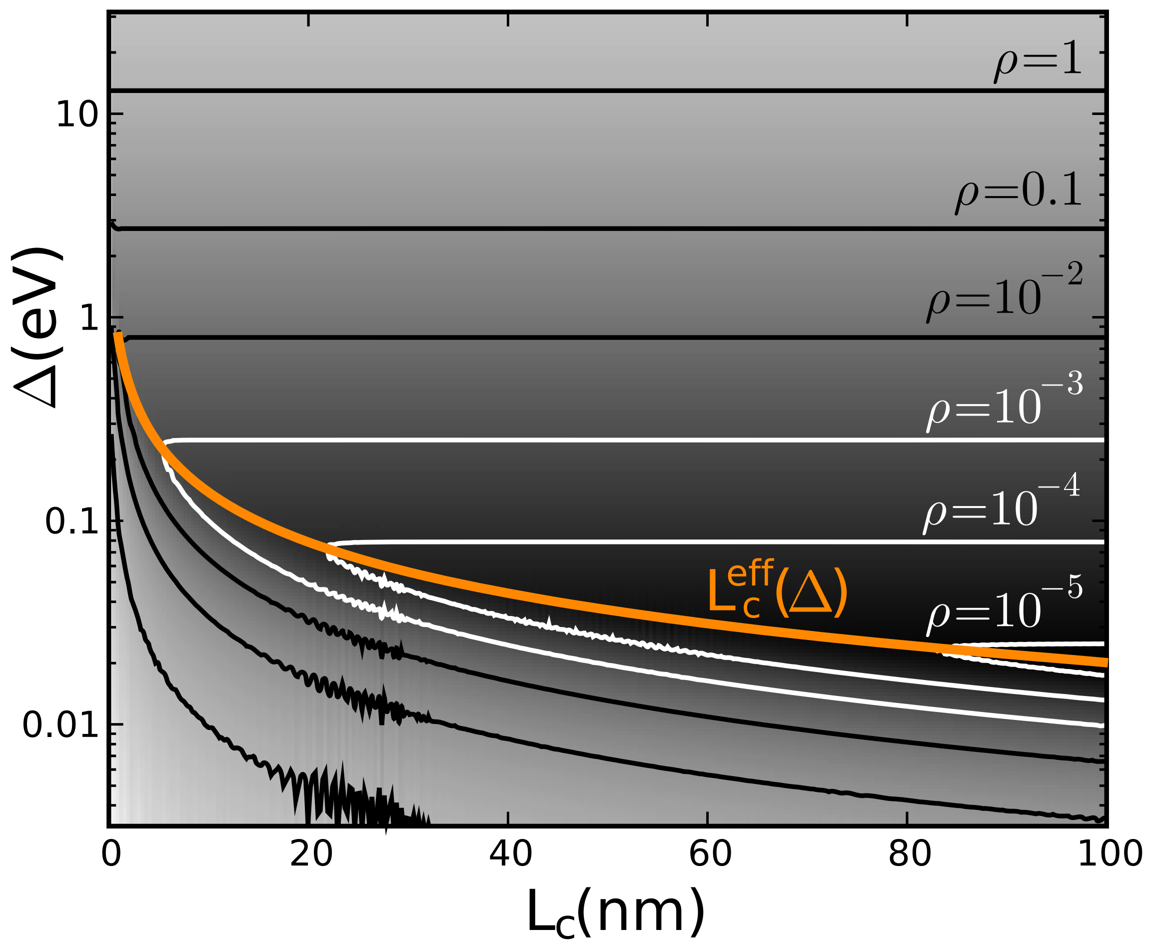


Effective contact length $L^{\mathrm{c}}_{\mathrm{eff}}(\Delta)$

For $L_{\mathrm{c}} > L^{\mathrm{c}}_{\mathrm{eff}}$: contact reflection saturates at $\rho_{\min}(\Delta)$

Effective contact length L^{c}_{eff}





strong coupling regime:

$$\rho_s(\Delta) = c_1 \Delta^2$$

weak coupling regime:

$$\rho_w(L_c, \Delta) = c_2 \exp\left(-\frac{L_c \Delta}{c_3}\right)$$

border of both regimes:

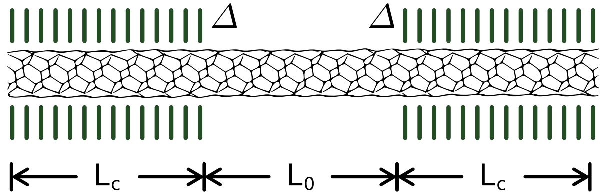
$$\rho_w(L^{c}_{eff}(\Delta), \Delta) \;=\; \rho_s(\Delta)$$

$$\Rightarrow \quad L^{c}_{eff}(\Delta) \;=\; \ell_{uc} \frac{\alpha_1}{\Delta} \ln \frac{\alpha_2}{\Delta}$$

with the length of the unit cell $\ell_{uc} = 0.25\,\mathrm{nm}$

numerical fit gives: $\alpha_1 = 1.32\,\mathrm{eV}$, $\alpha_2 = 9.14\,\mathrm{eV}$

Putting it together



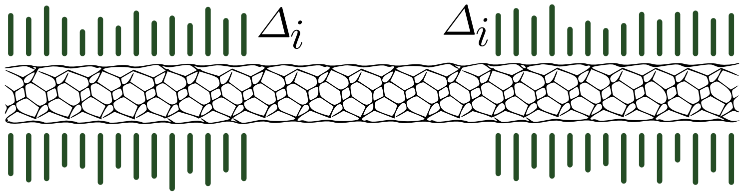
	Pd	Ti
$\Delta = \left(\gamma_{\substack{\text{carbon}\\ \text{metal}}}\right)^2 \times \text{LDOS}_{\text{metal-surface}}$	0.02 eV	0.1 eV
$L^{\text{c}}_{\text{eff}} = \ell_{\text{uc}} \frac{\alpha_1}{\Delta} \ln \frac{\alpha_2}{\Delta}$	$\sim 30\,\text{nm}$	$\sim 4\,\text{nm}$

Effective scattering region longer than uncovered region:

$$L_0 < L_0^{\text{eff}} < L_0 + 2L^{\text{c}}_{\text{eff}}$$

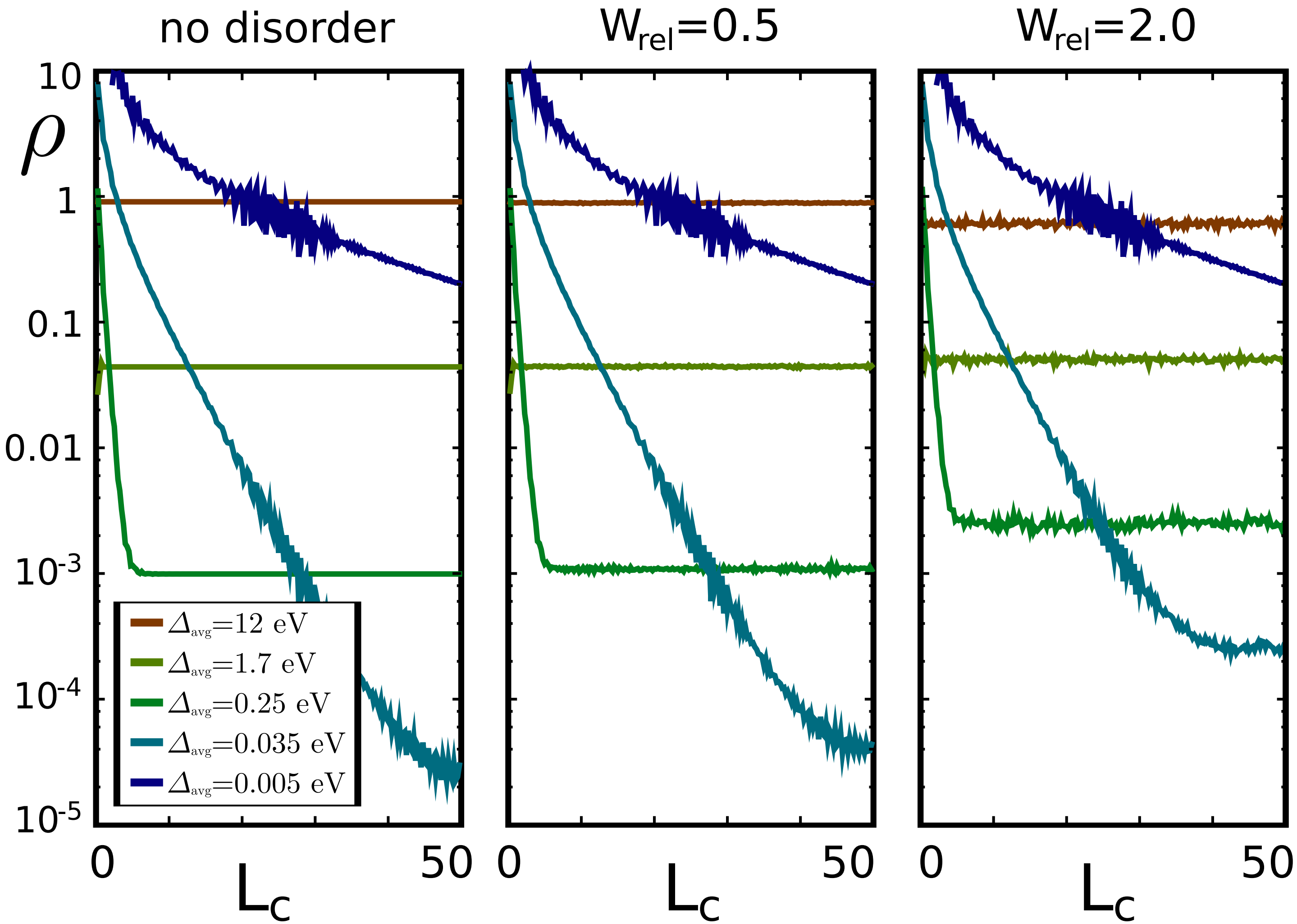
$\longrightarrow$ Fabry-Perot ?

Nonepitaxial interfaces

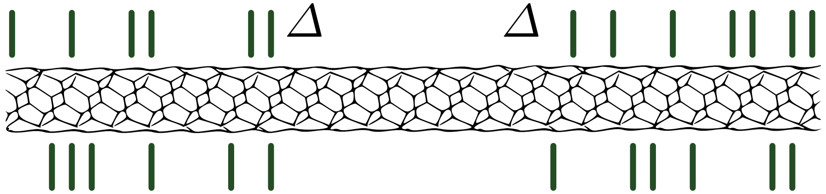


Model 1: disordered contacts

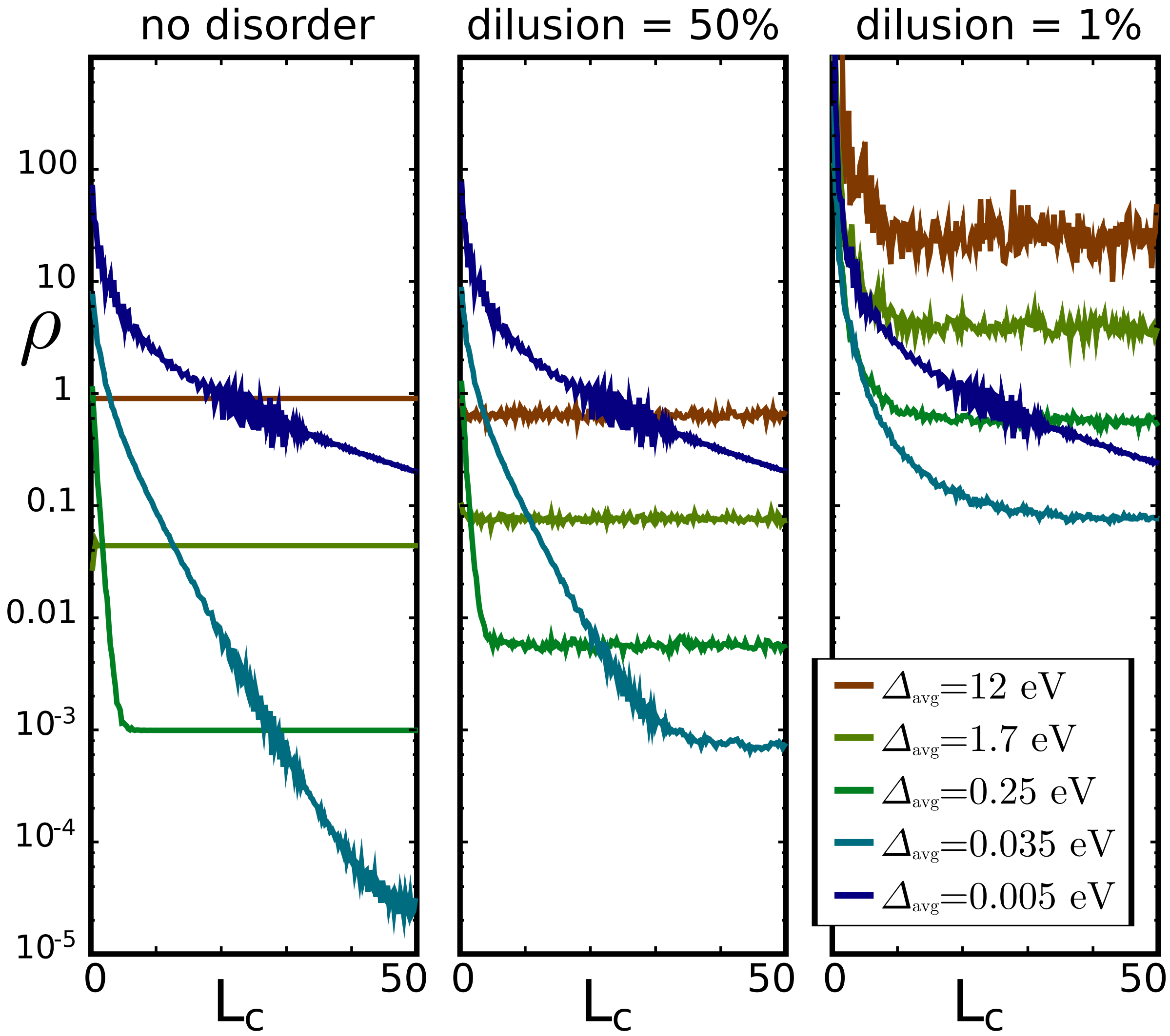
$\Delta_i \in [(1 - W_{\text{rel}})\Delta_{\text{avg}}; (1 + W_{\text{rel}})\Delta_{\text{avg}}]$ (uniform random distribution)



Nonepitaxial interfaces



Model 2: diluted contacts



Summary

- realistic (ab initio) description of the metal/CNT interface
- effective TB hamiltonian for the CNT + contact system
- *weak coupling (poor metal) + long contact*
  $\longrightarrow$ *optimal charge injection*
- *enhanced effective scattering region*
- effect robust against disorder at the interface

Outlook

- more on disorder, more detailed microscopic modelling
- charge-transfer (selfconsistent calculation)
- ferromagnetic contacts ($\longrightarrow$ *spin transport*)
- superconducting contacts