Charge transport through gated DNA; role of the helical confirmation

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E. Martz, Uni. of Massachusetts: http://molvis.sdsc.edu/dna/
A. Herráez, Uni. of Alcalá: biomodel.uah.es/en/model4/dna/

Outline

The DNA structure

Conductivity of the DNA

Modeling the gated DNA; the helical geometry

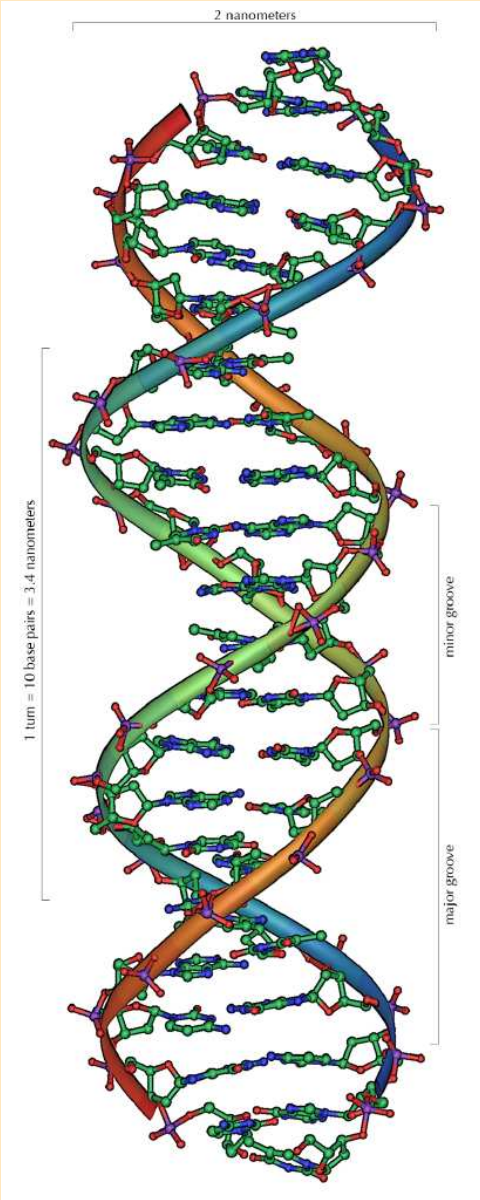
Current-voltage characteristics; strong gating effect

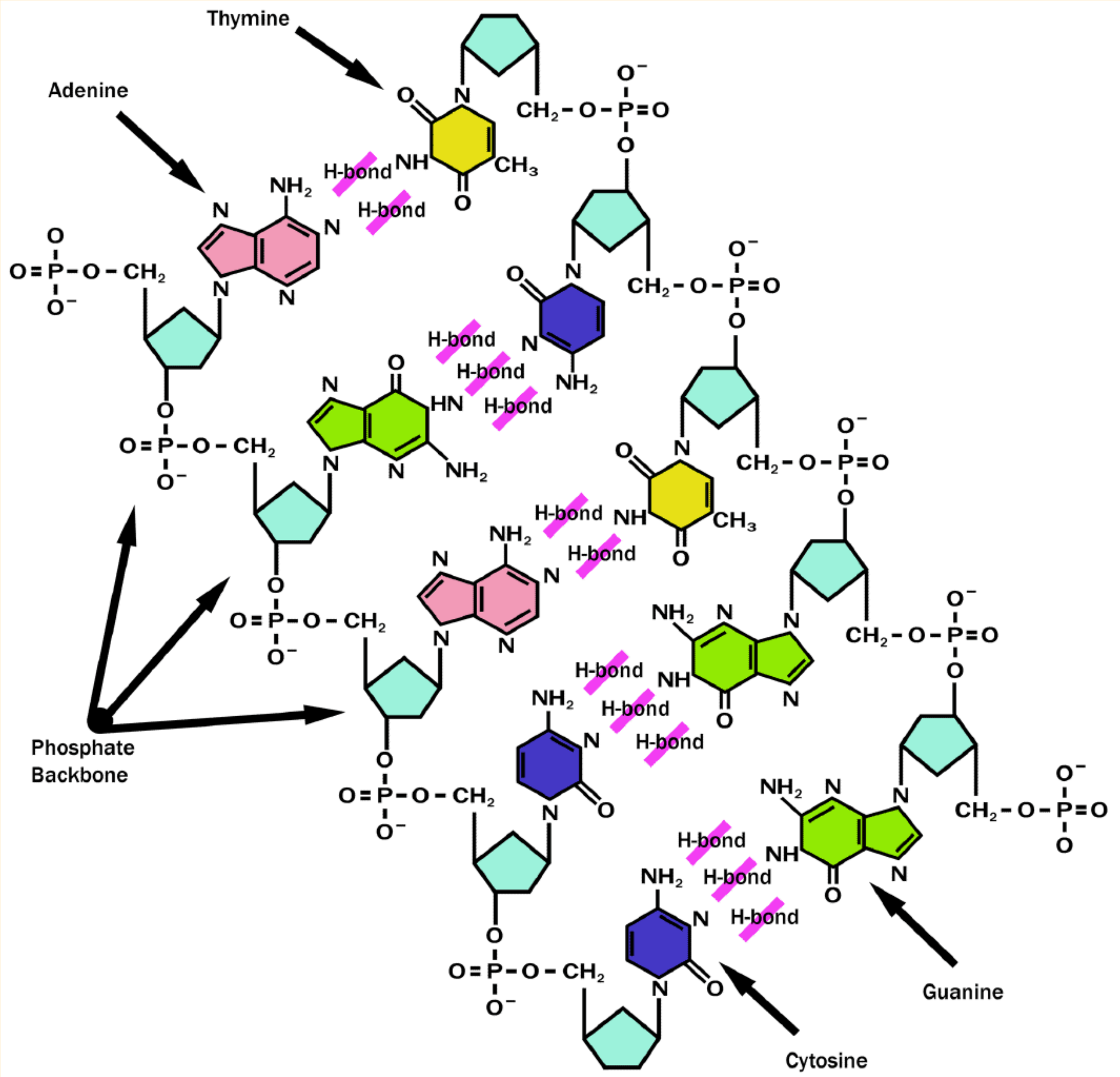
Possible applications for single molecule devices

Proposed experimental set-ups

Summary

The structure of the DNA





Conductivity of the DNA

insulating: 5 publications

Conductivity of the DNA

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semiconducting: 6 publications

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metallic: 6 publications

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metallic: 6 publications

superconducting: 1

Conductivity of the DNA

insulating: 5 publications

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metallic: 6 publications

superconducting: 1

Factors affecting the conductivity:

- environment / DNA form
- base sequence

Base sequences

random correlated (natural DNA) $\Rightarrow$ insulator

periodic (synthetic DNA) $\Rightarrow$ semiconductor

Synthetic DNA:

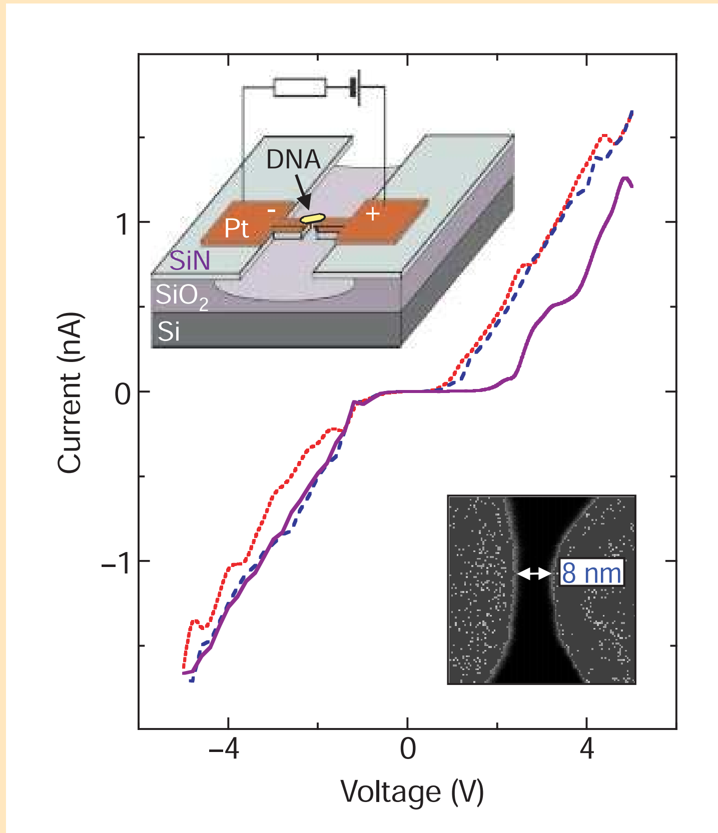
- poly(A)-poly(T)
- poly(G)-poly(C)

Semiconducting poly(G)-poly(C) DNA

Direct measurement of electrical transport through DNA molecules

Danny Porath*, Alexey Bezryadin*†, Simon de Vries* & Cees Dekker*

** Department of Applied Sciences, Delft University of Technology, 2628 CJ Delft The Netherlands*



D. Porath, A. Bezryadin, S. de Vries, C. Dekker, *Nature* **403**, 635 (2000)

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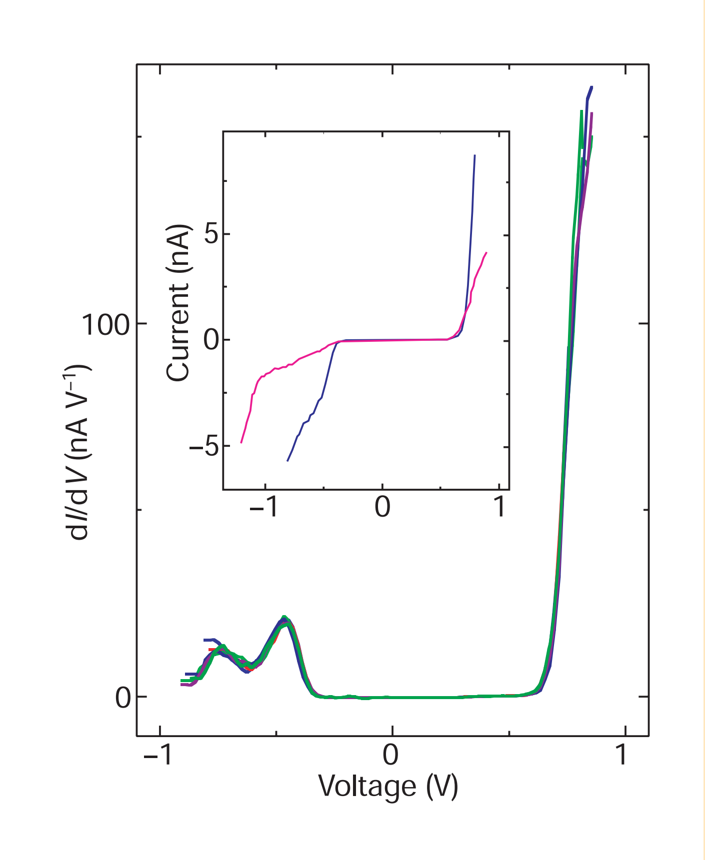
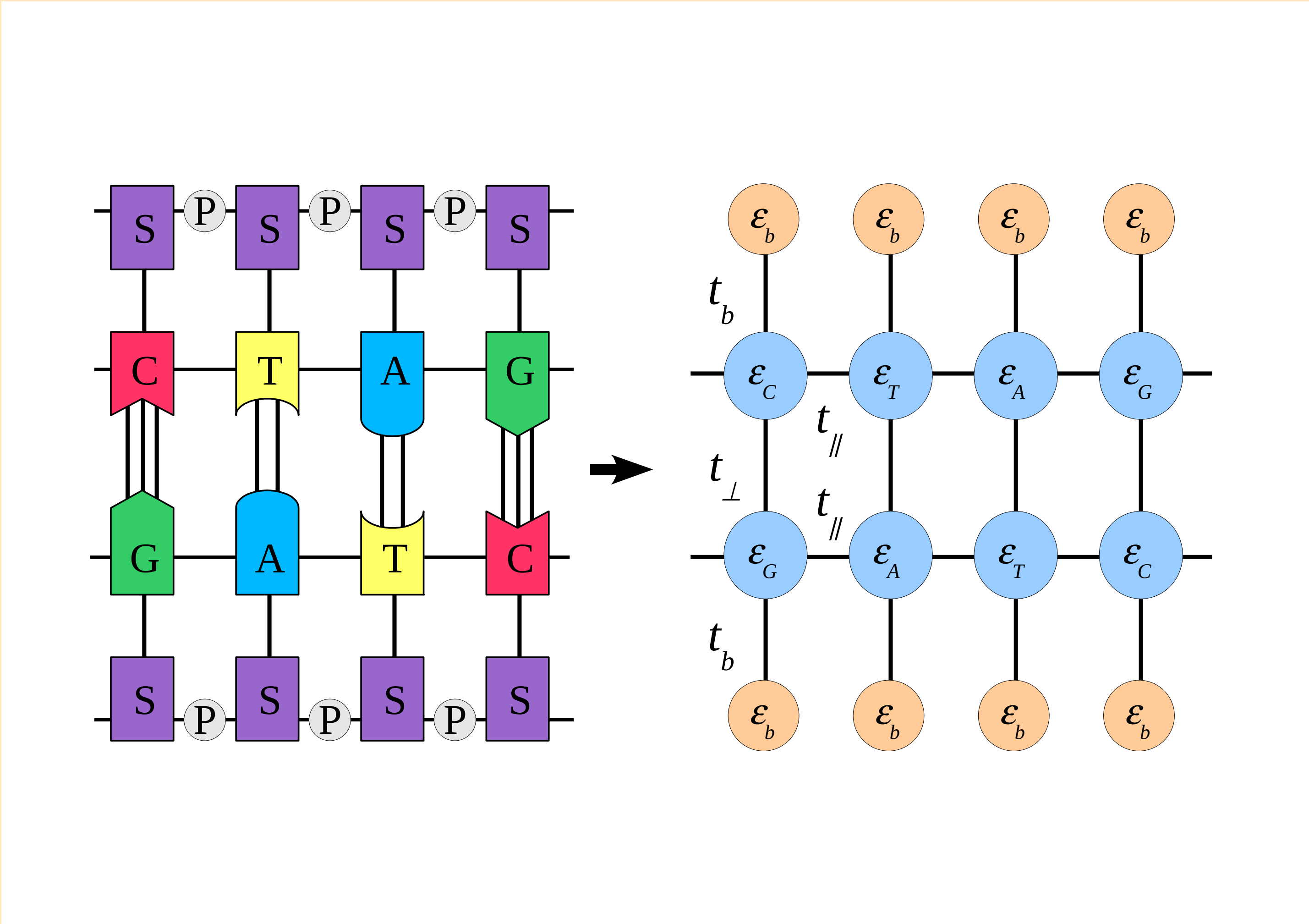


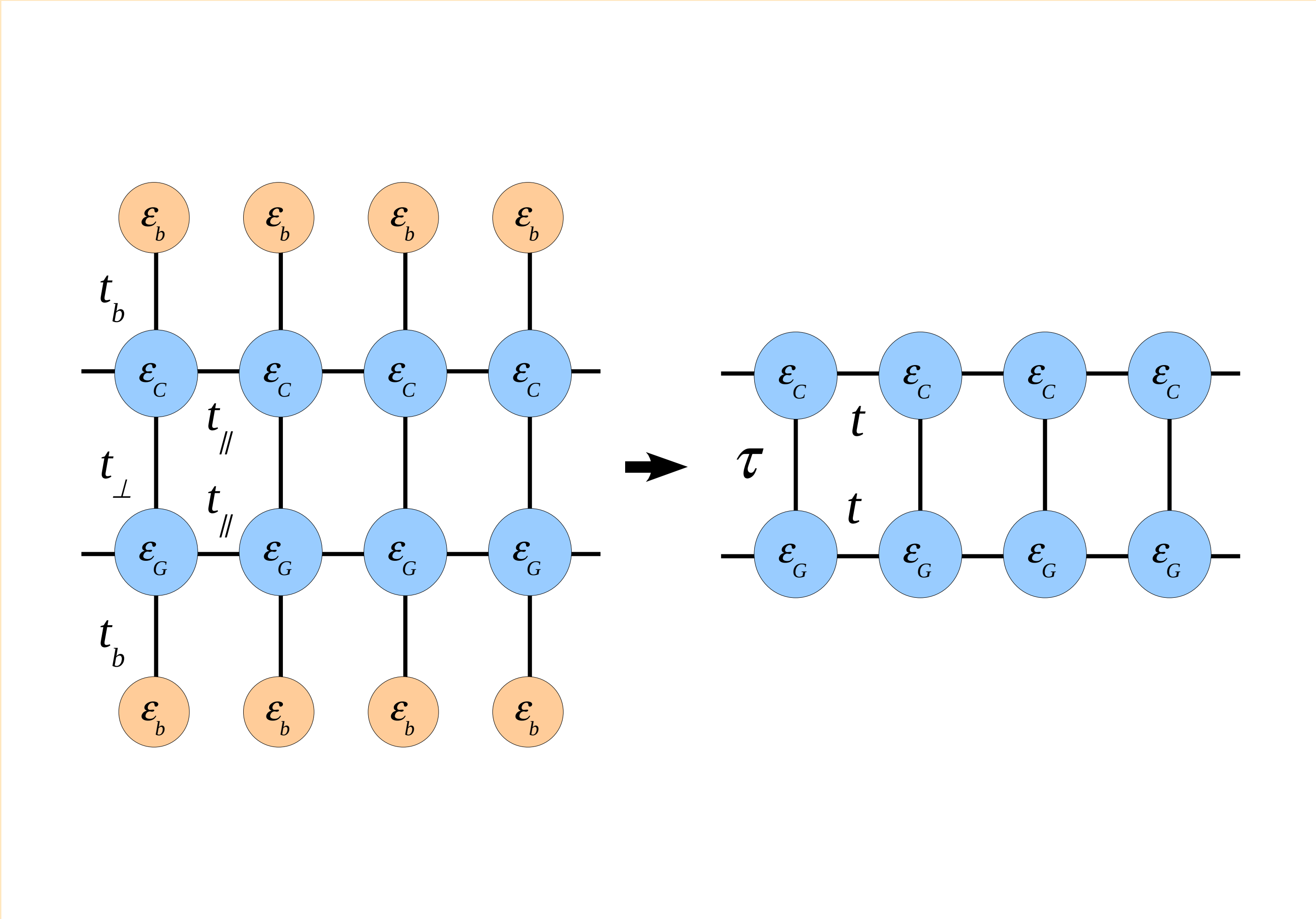
D. Porath, A. Bezryadin, S. de Vries, C. Dekker, *Nature* **403**, 635 (2000)

DNA models: dangling backbone ladder model

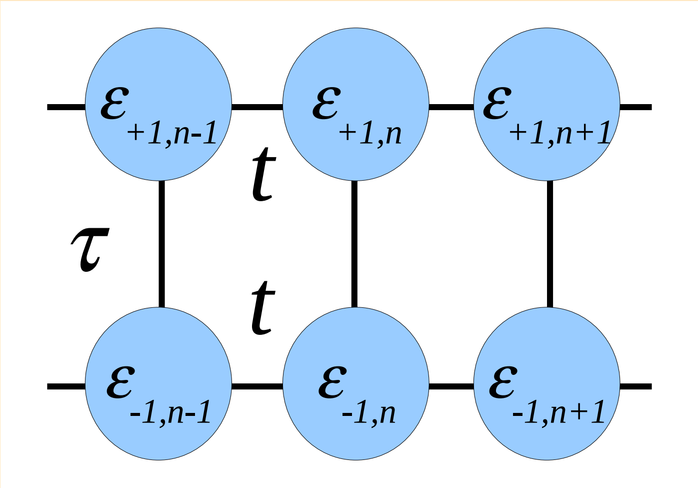


D. Klotsa, R. A. Römer, and M. S. Turner, Biophys. J. **89**, *2187 (2005)*

Poly(G)-poly(C) DNA: the ladder model



The minimum ladder model



$$\hat{H}_{DNA} = \sum_{n,s=\pm 1} \left(\varepsilon_{sn} b^{\dagger}_{sn} b_{sn} - t\, b^{\dagger}_{sn+1} b_{sn} + h.c. - \tau\, b^{\dagger}_{-sn} b_{sn} \right)$$

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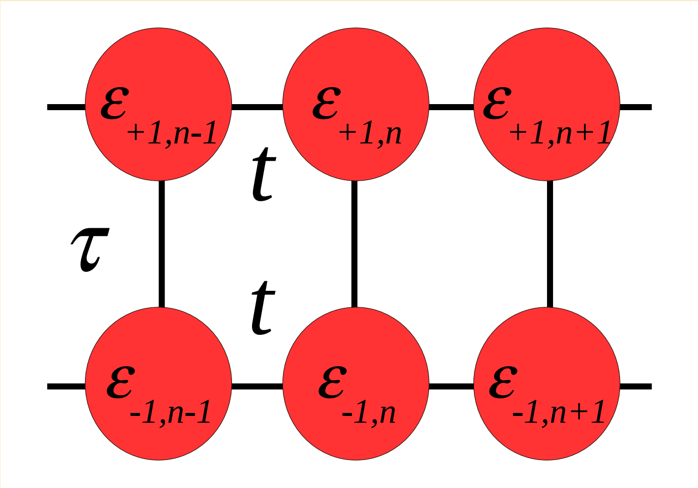

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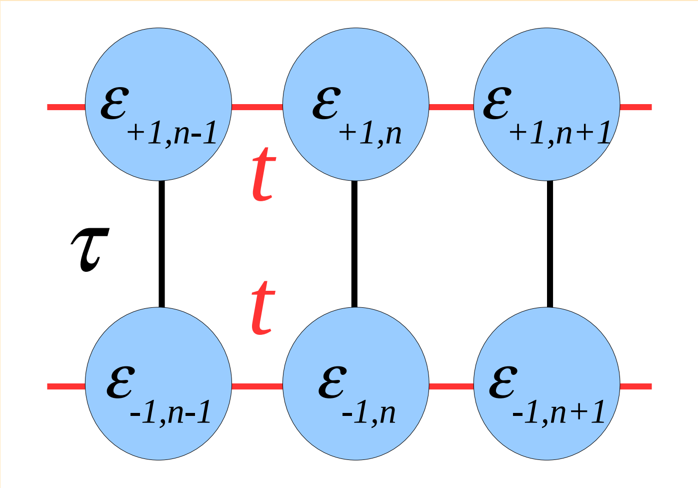

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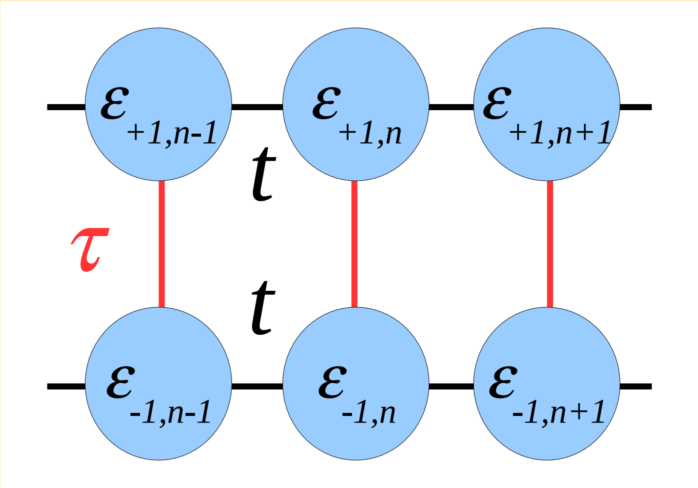
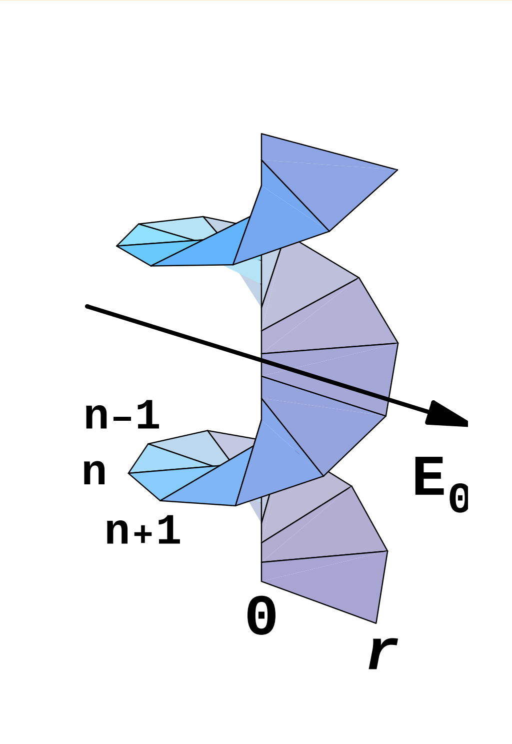


$$\hat{H}_{DNA} = \sum_{n,s=\pm 1} \left(\varepsilon_{sn} b_{sn}^{\dagger} b_{sn} - t\, b_{sn+1}^{\dagger} b_{sn} + h.c. - \tau\, b_{-sn}^{\dagger} b_{sn} \right)$$

[*K. Iguchi, Int. J. Mod. Phys. B* **11**, *2405 (1997)*]

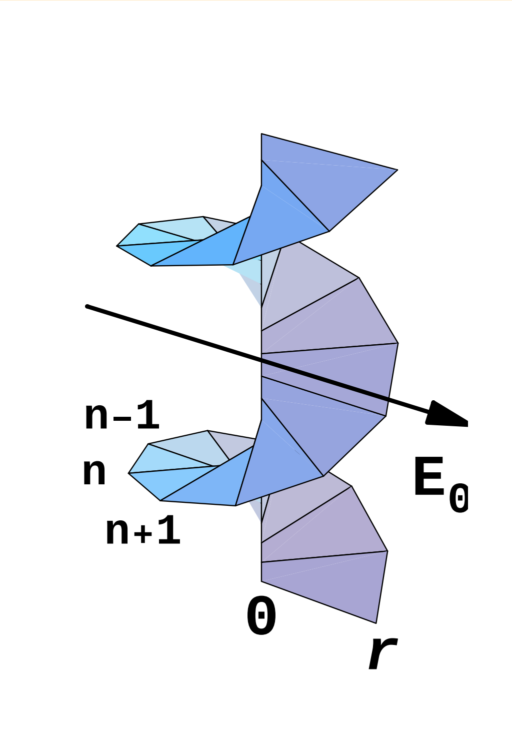
Helical geometry: modeling the gated DNA



$$\varepsilon_{sn} = \varepsilon_{sn}^{(0)} + s\, e\, \frac{V_g}{2} \cos\left(\frac{2\pi n}{10} + \varphi_0\right)$$

$$V_g = 2E_0\, r, \quad s = \pm 1$$

Helical geometry: modeling the gated DNA



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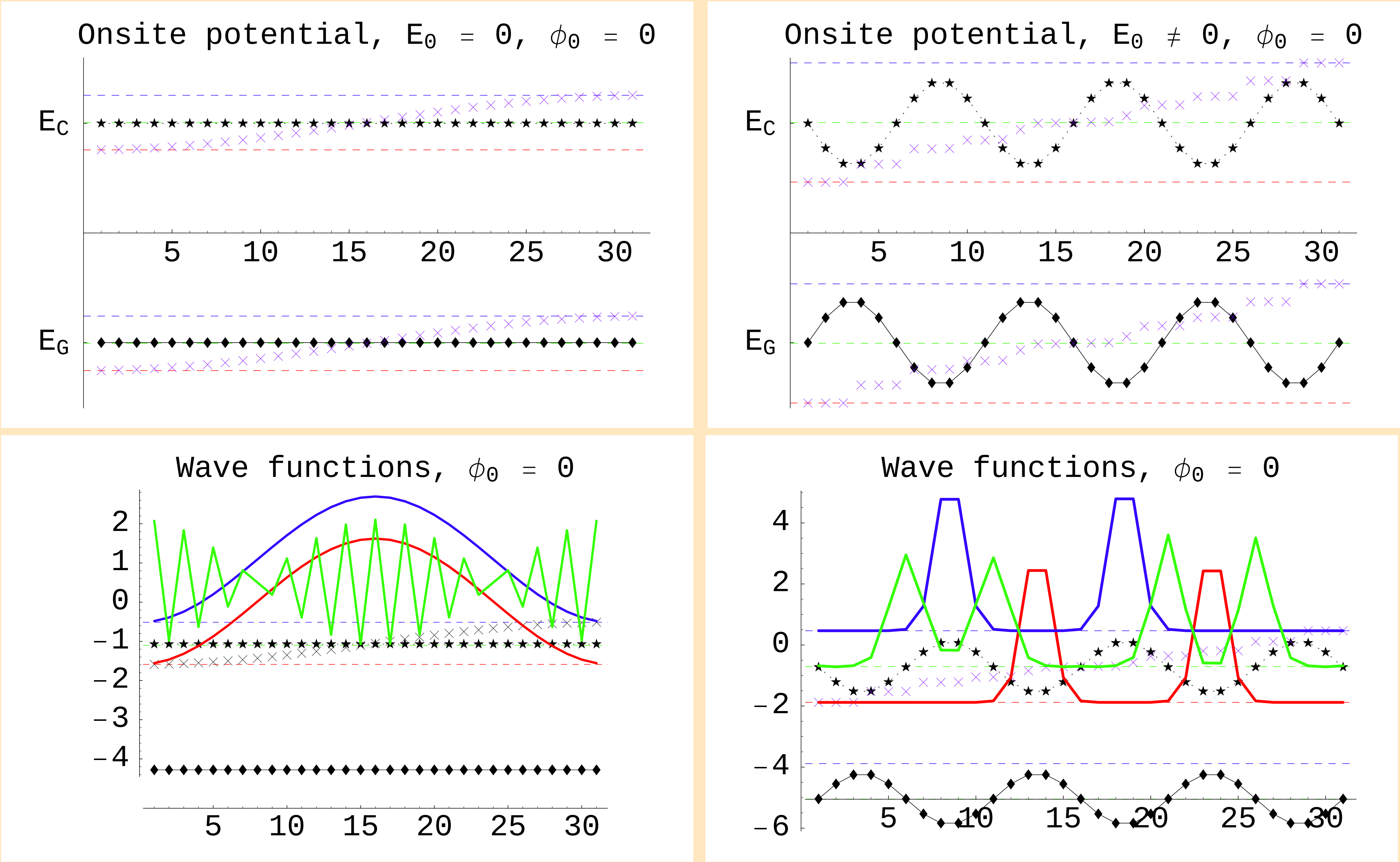
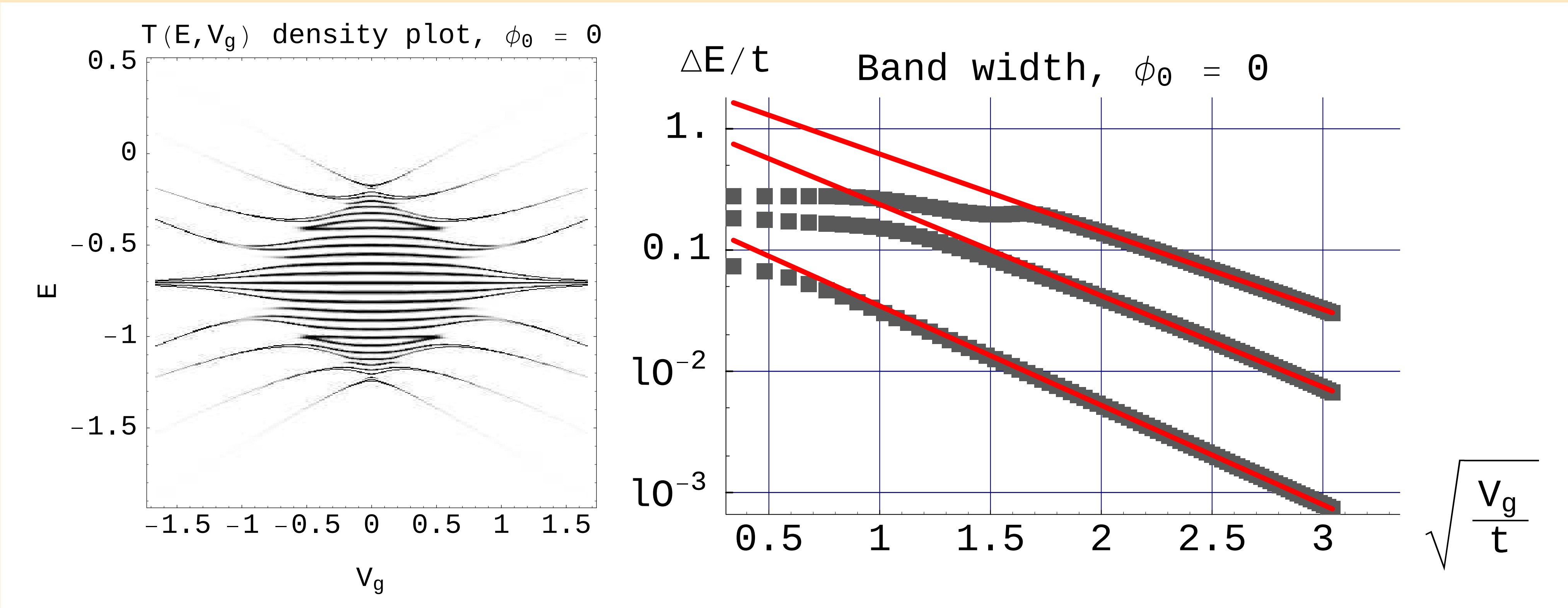
Site potential profile

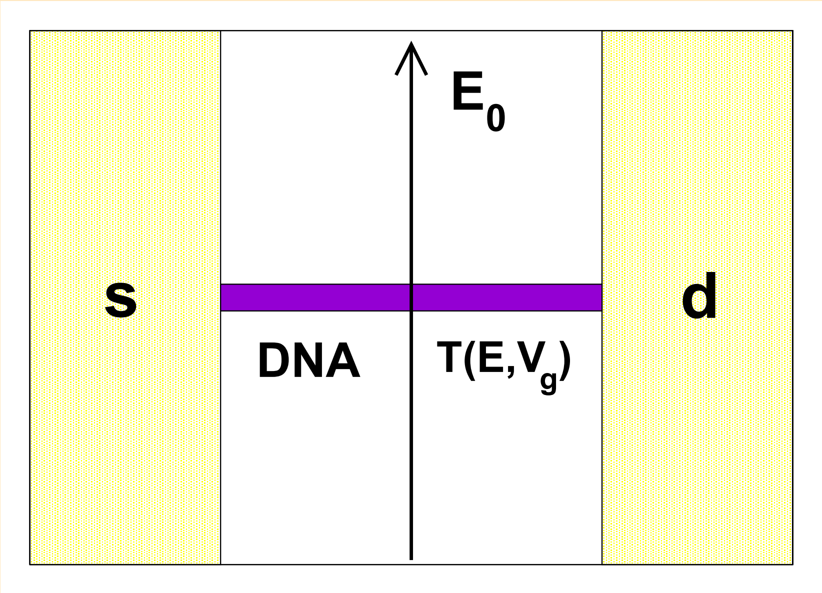


Mini-band width



$$\Delta E \sim \exp\left(-\alpha\, N \sqrt{\frac{V_g}{t}}\right)$$

The ladder model + contacts



$$\hat{H} = \hat{H}_{DNA} + \hat{H}_{el} + \hat{H}_{DNA-el}$$

$$\hat{H}_{DNA} = \sum_{s,n} \left(\varepsilon_{sn} b^{\dagger}_{sn} b_{sn} - t\, b^{\dagger}_{sn+1} b_{sn} + h.c. - \tau\, b^{\dagger}_{-sn} b_{sn} \right)$$

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$$\hat{H}_{DNA-el} = \sum_{s} \left(-\Gamma_{sl}\, c^{\dagger}_{s0} b_{s1} - \Gamma_{sr}\, c^{\dagger}_{sN+1} b_{sN} + h.c. \right)$$

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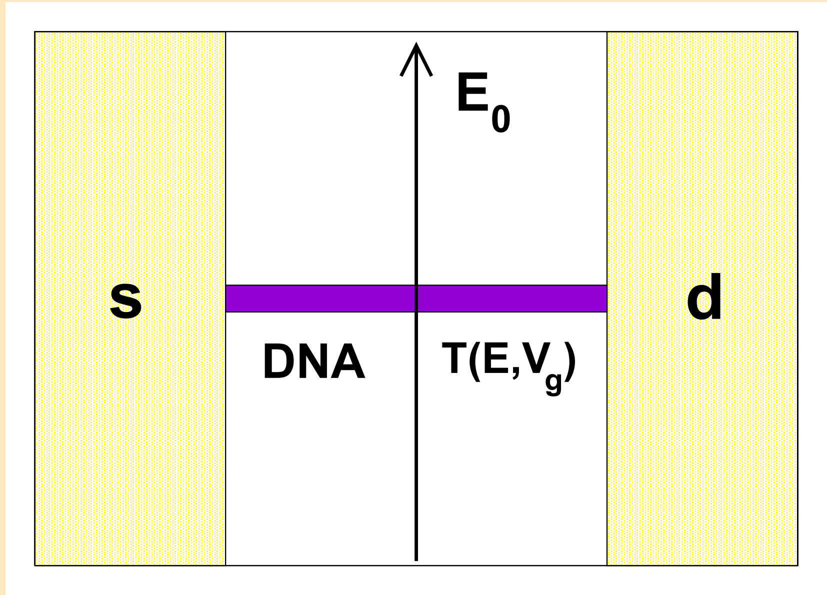

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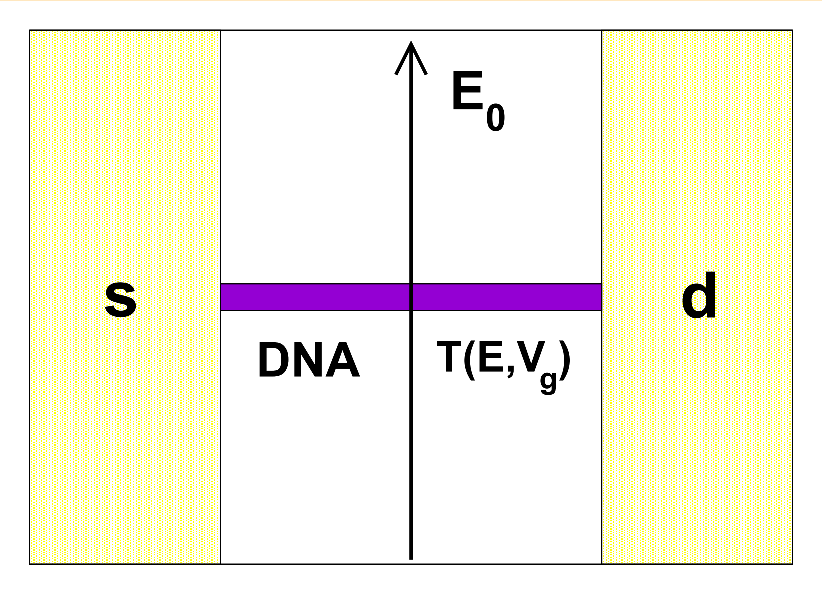

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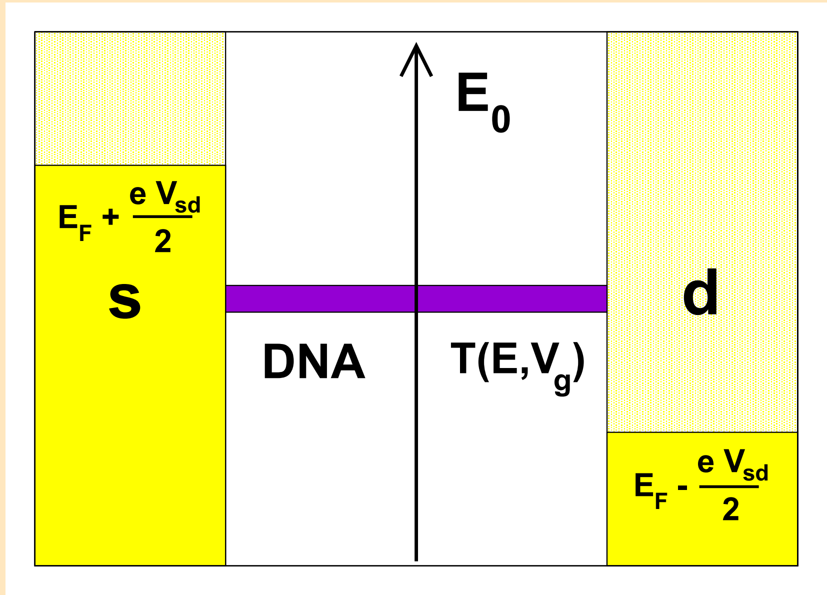
Calculating current-voltage characteristics



$$I(V_g, V_{sd}) = \frac{2e}{h} \int T(V_g, E) \left[f_l(E, V_{sd}) - f_r(E, V_{sd}) \right] dE$$

$$f_{l,r}(E, V_{sd}) = \frac{1}{1 + e^{\frac{E_F \pm eV_{sd}/2 - E}{kT}}}$$

- $T(V_g, E)$ is the transmission coefficient
- V_{sd} and V_g source-drain and gate voltages
- $E_F = 0$ is the Fermi energy at equilibrium

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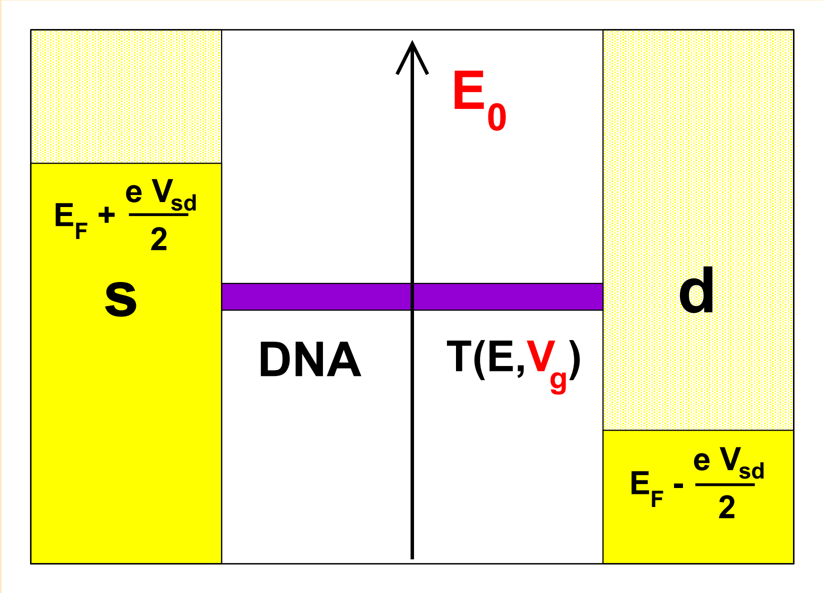

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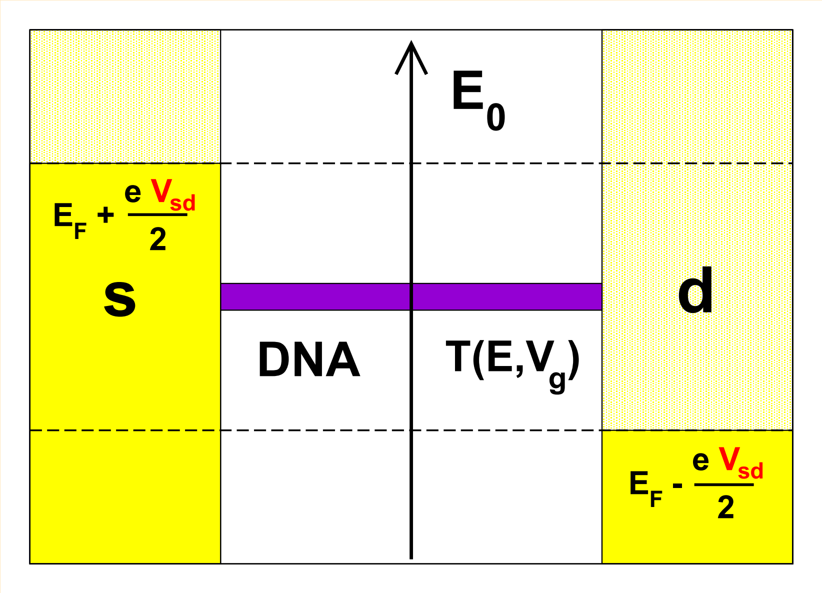

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Poly(G)-poly(C) DNA: parameters

- $N = 31$ ($L \approx 10.5$nm), $T = 4K$

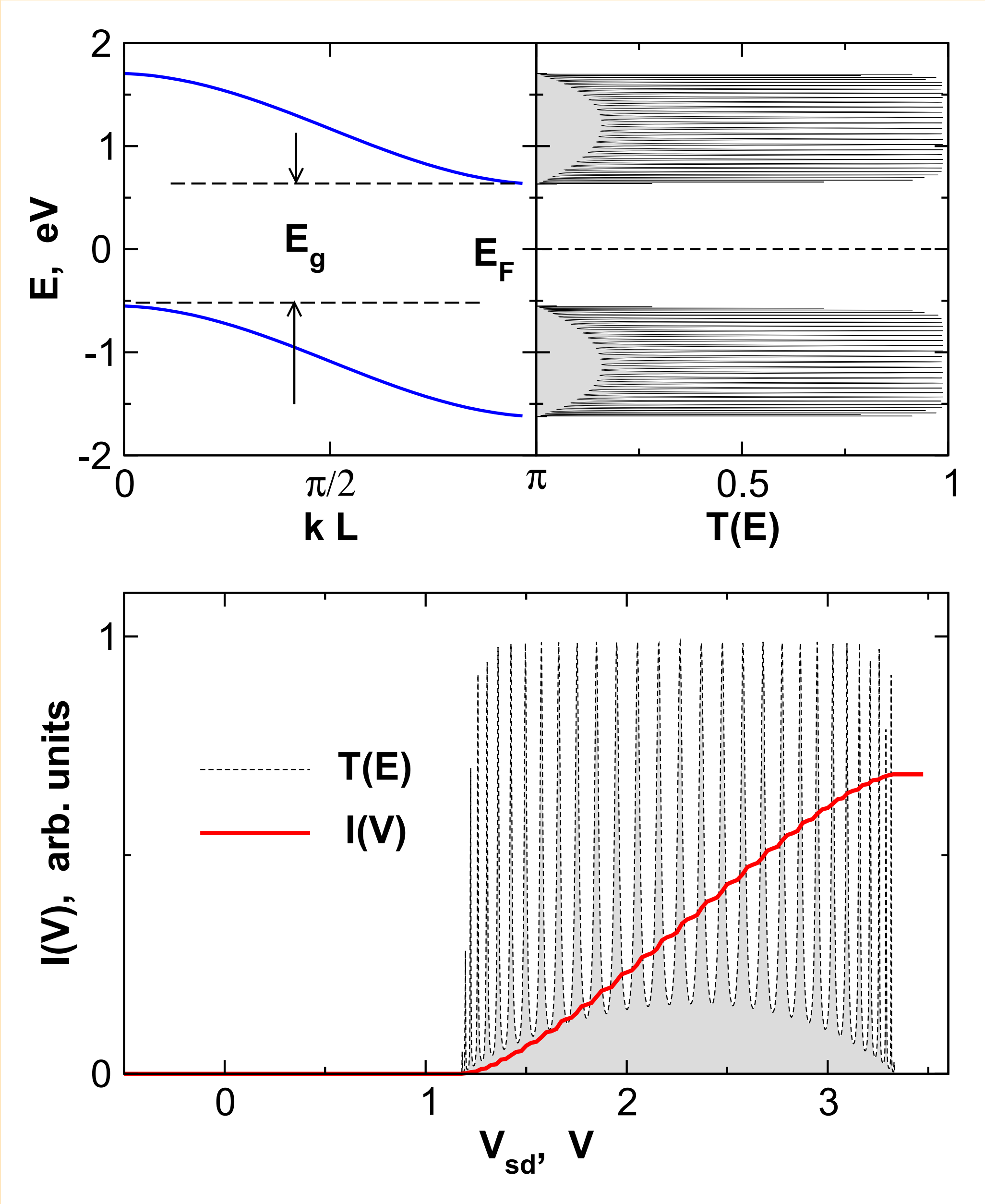
- $\varepsilon_G = 1.14eV$, $\varepsilon_C = -1.06eV$ *
- $t = 0.27eV$, $\tau = 0.25eV$ †

- $\varepsilon_{sM} = E_F = 0$, $t_M = 4\,t$ †
- $\Gamma_{sl} = \Gamma_{sr} = t$ †

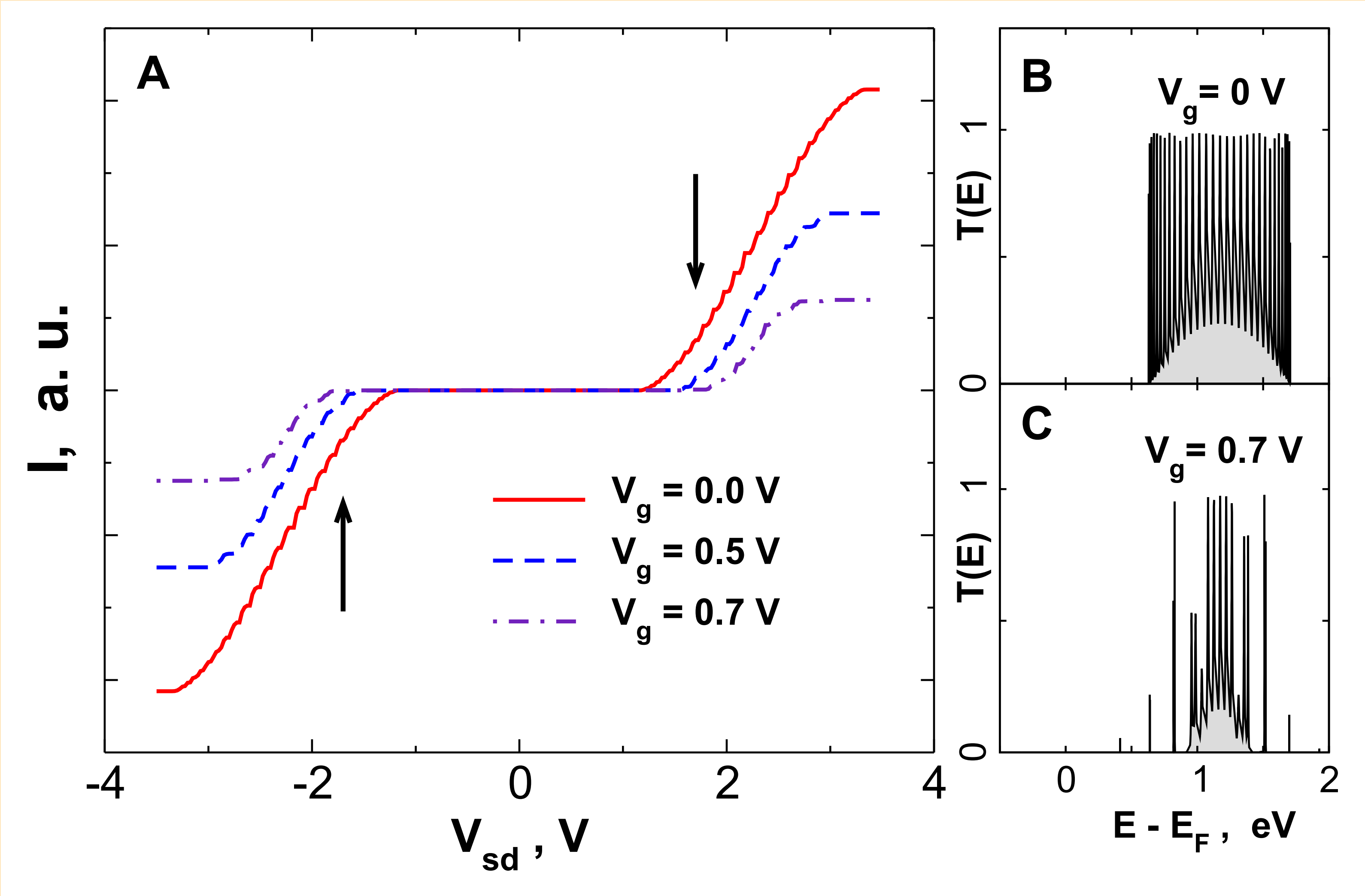
* H. Mehrez and M. P. Anantram, Phys. Rev. B **71**, 115405 (2005)

† R. Gutiérrez, S. Mohapatra, H. Cohen, D. Porath, and G. Cuniberti
Phys. Rev. B **74**, 235105 (2006)

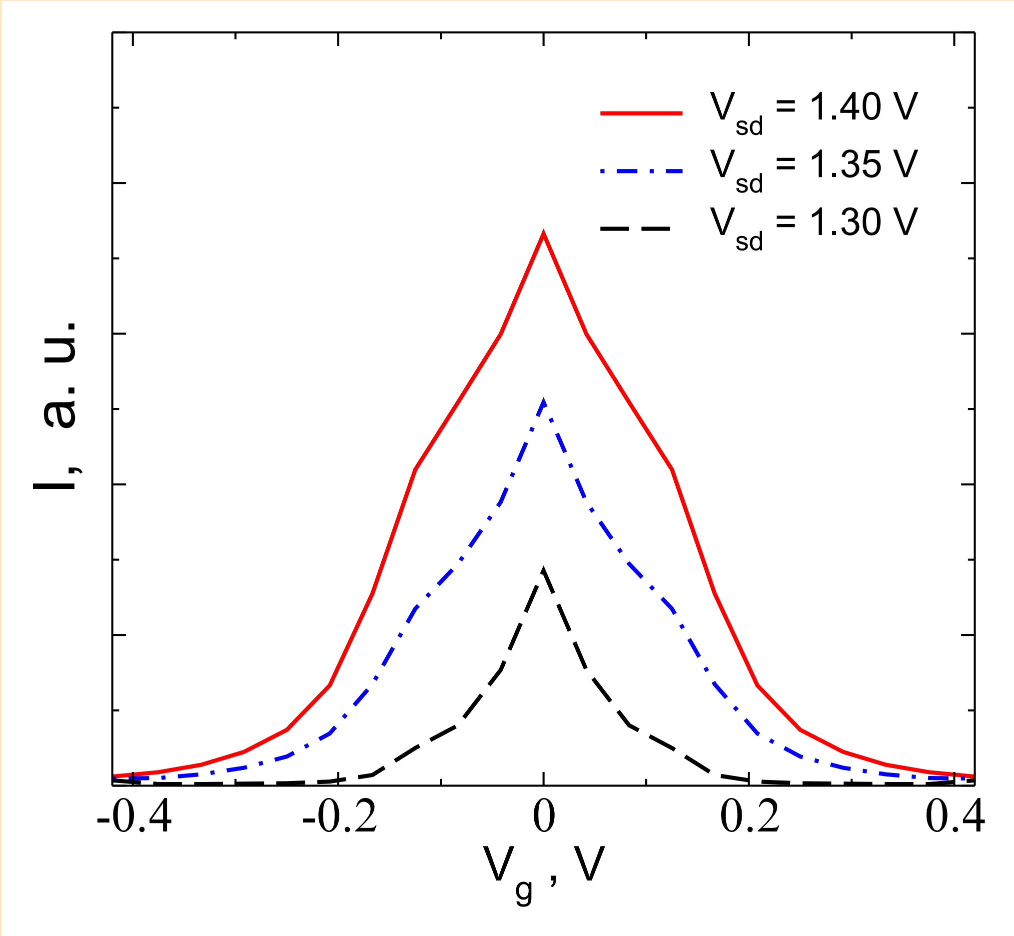
Poly(G)-poly(C) DNA: $E_0 = 0$



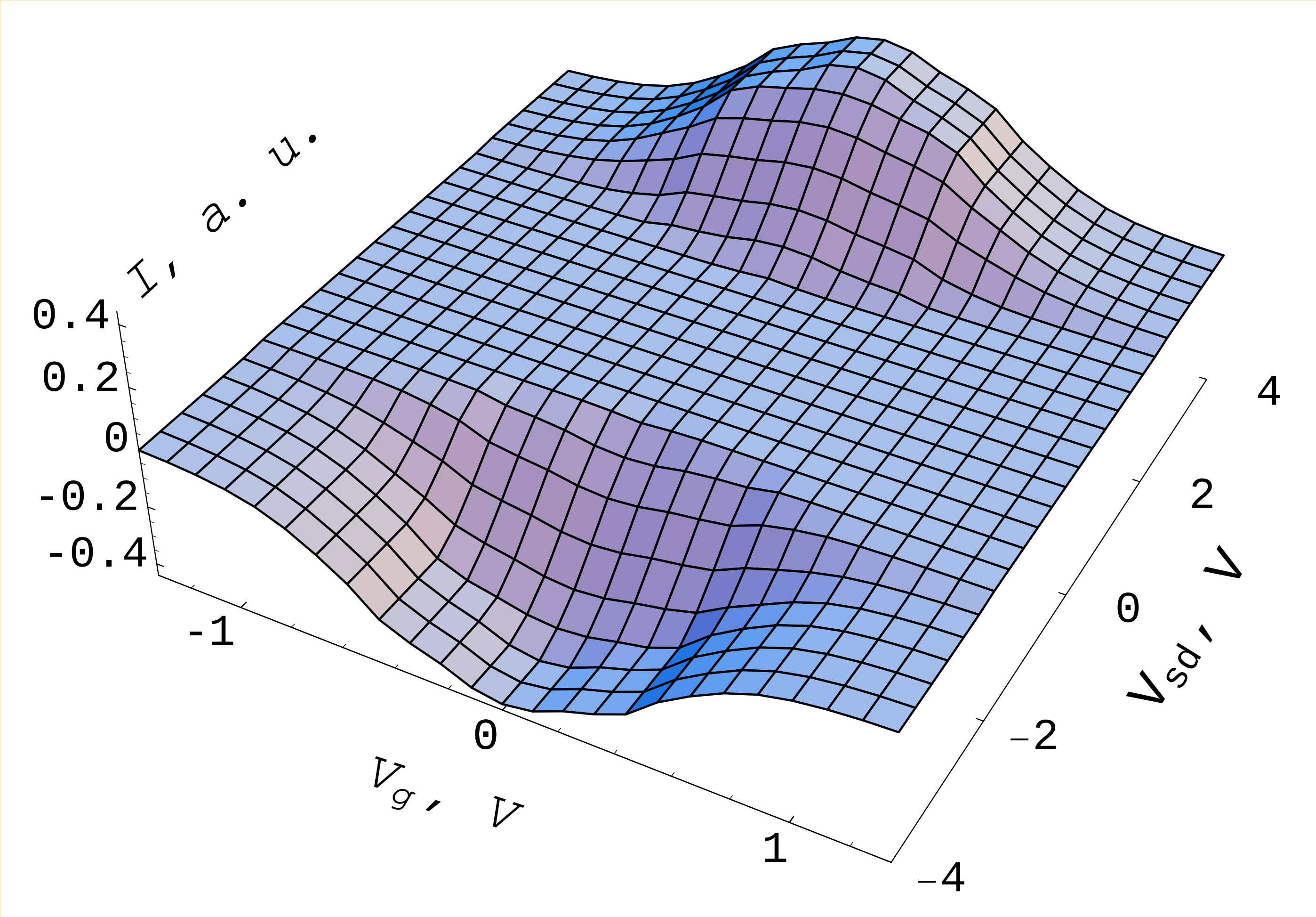
Gated poly(G)-poly(C) DNA: I-V curves



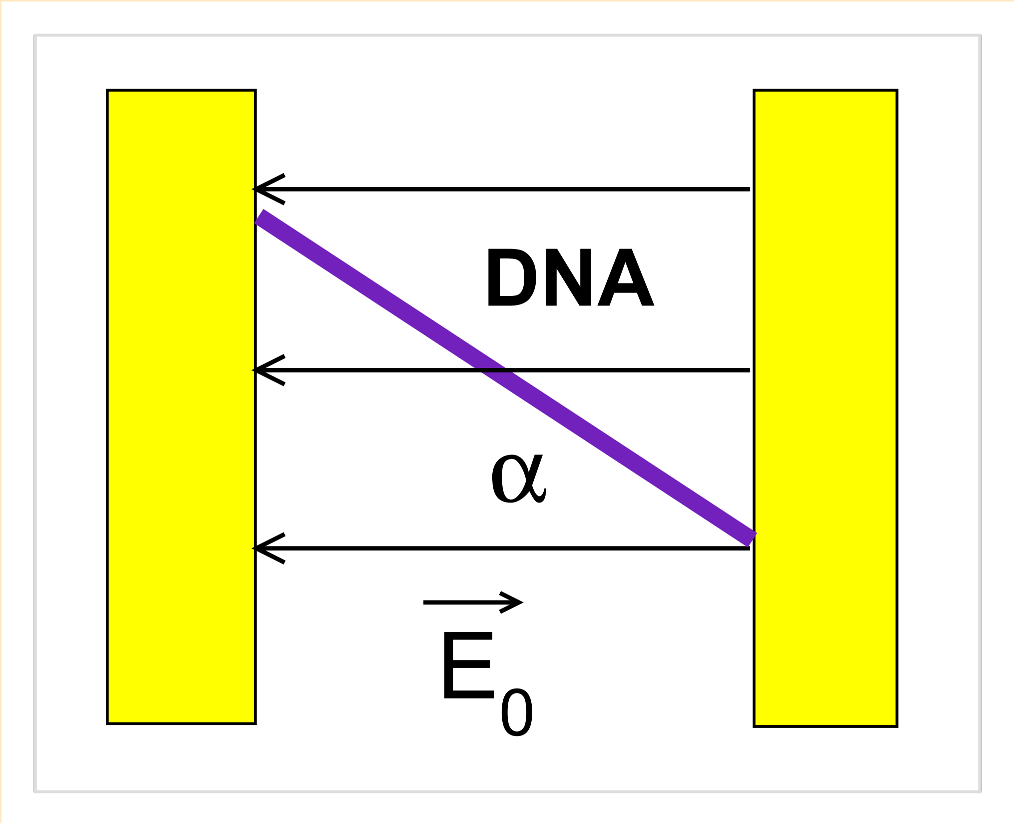
Poly(G)-poly(C) DNA: strong gating effect



Gated poly(G)-poly(C) DNA: I-V surface



Single molecule analog of the Esaki diode



$$V_g = \frac{2r}{L}\tan(\alpha)\,V_{sd}$$

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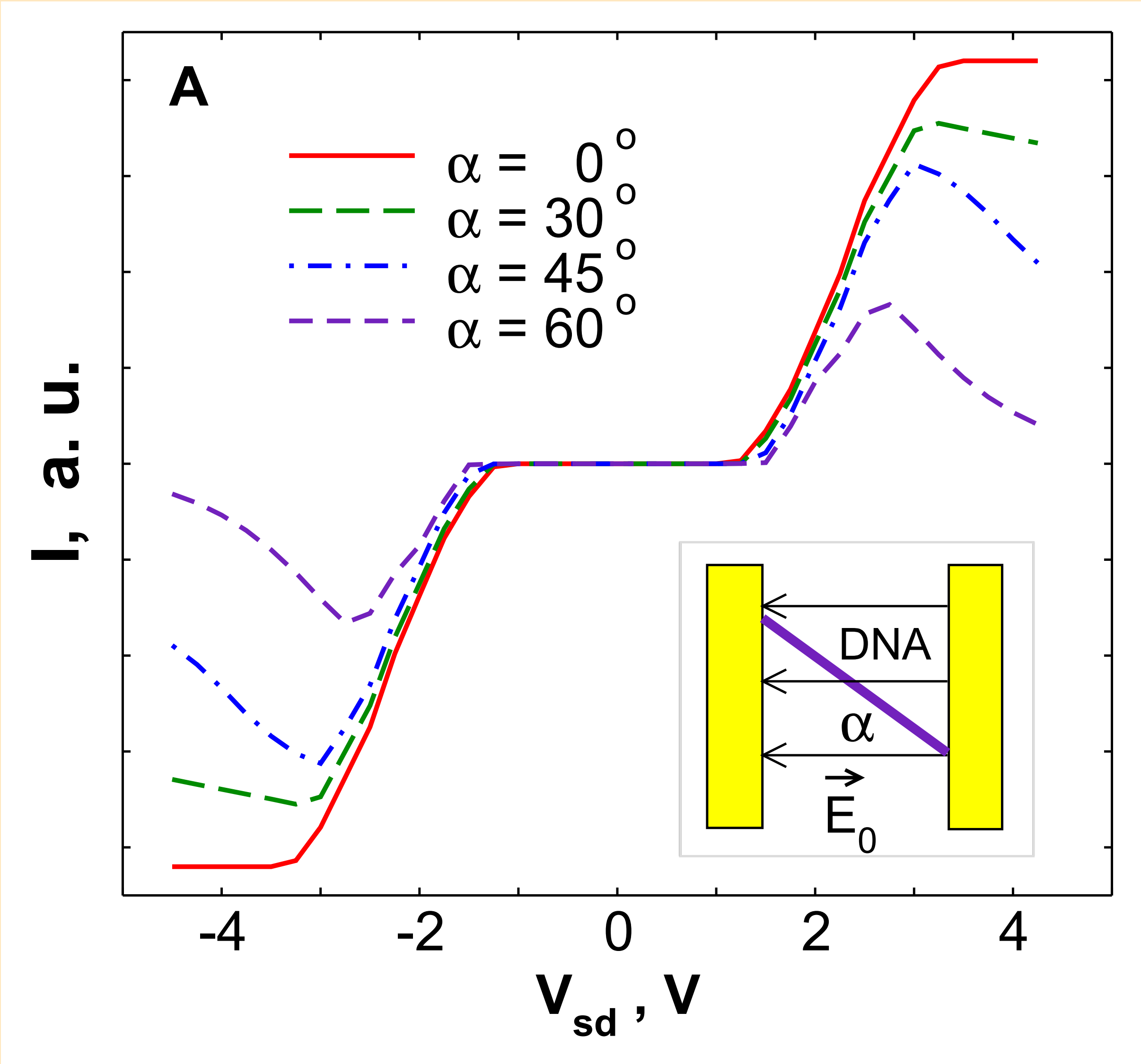
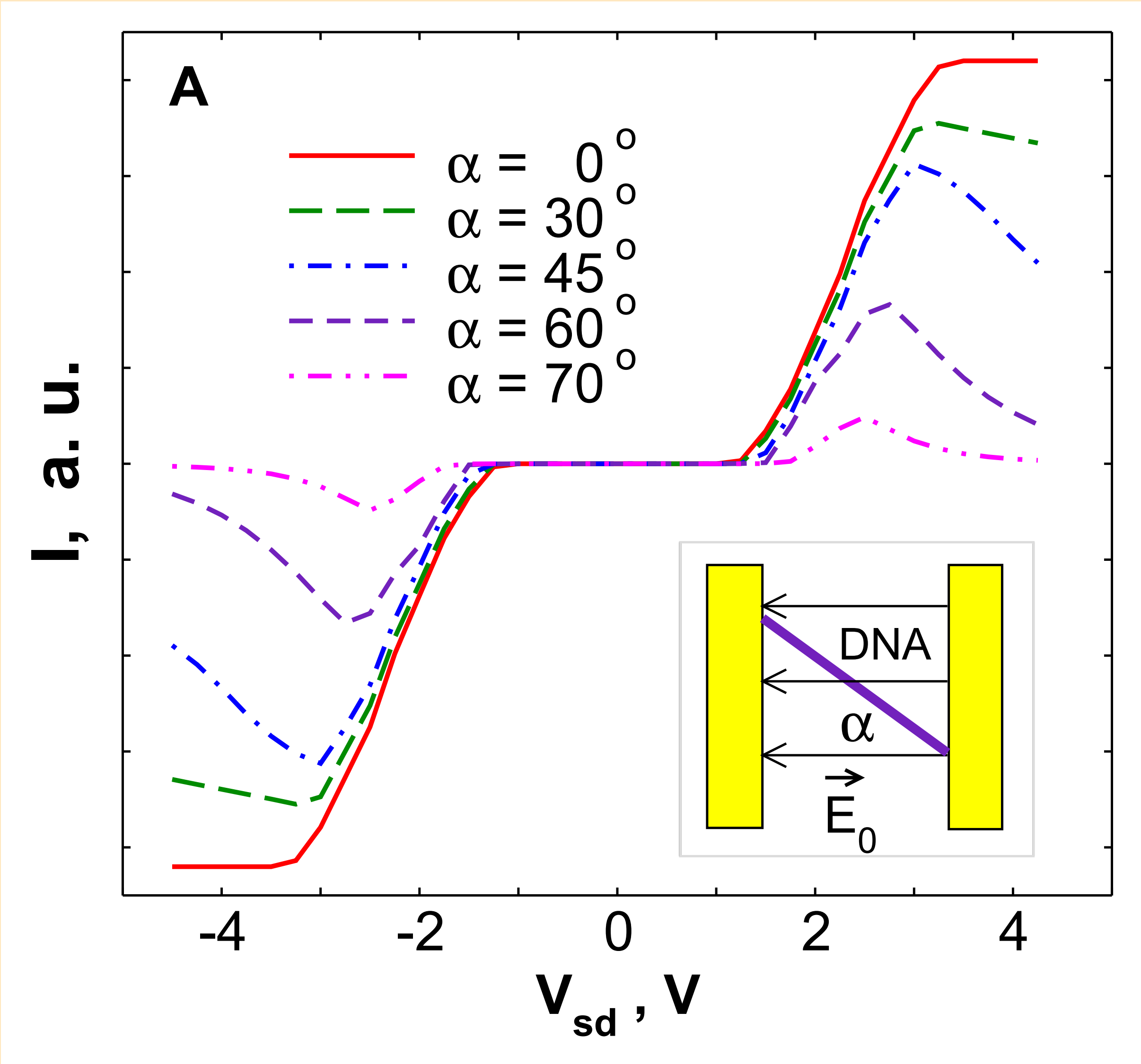
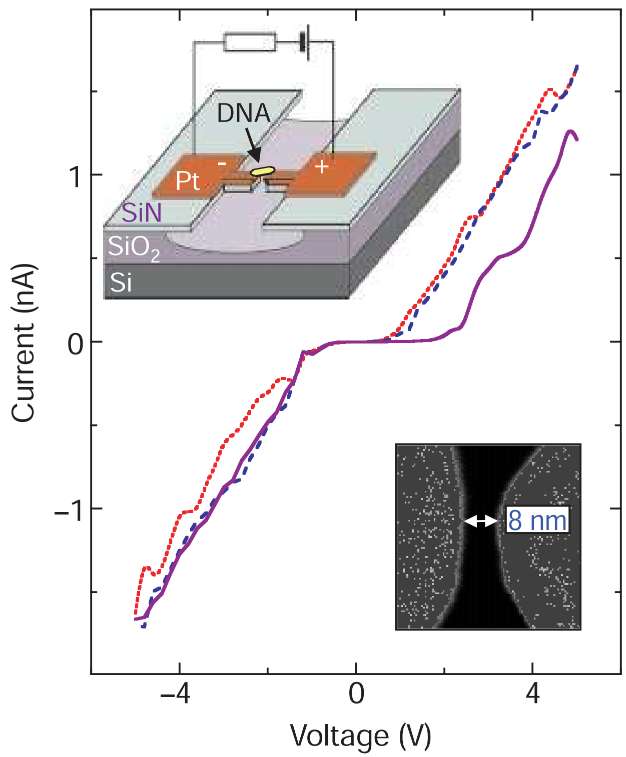
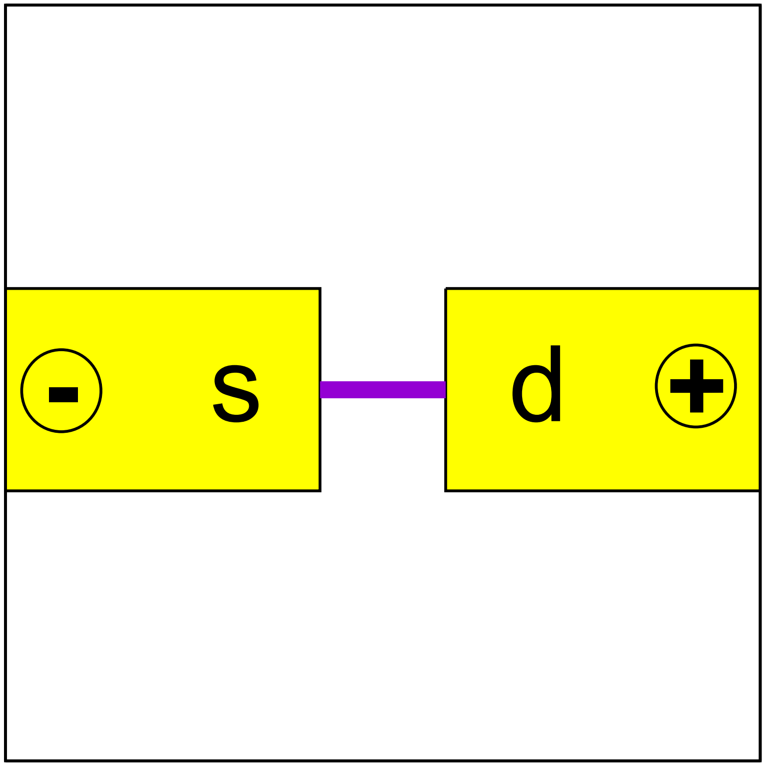


Single molecule analog of the Esaki diode

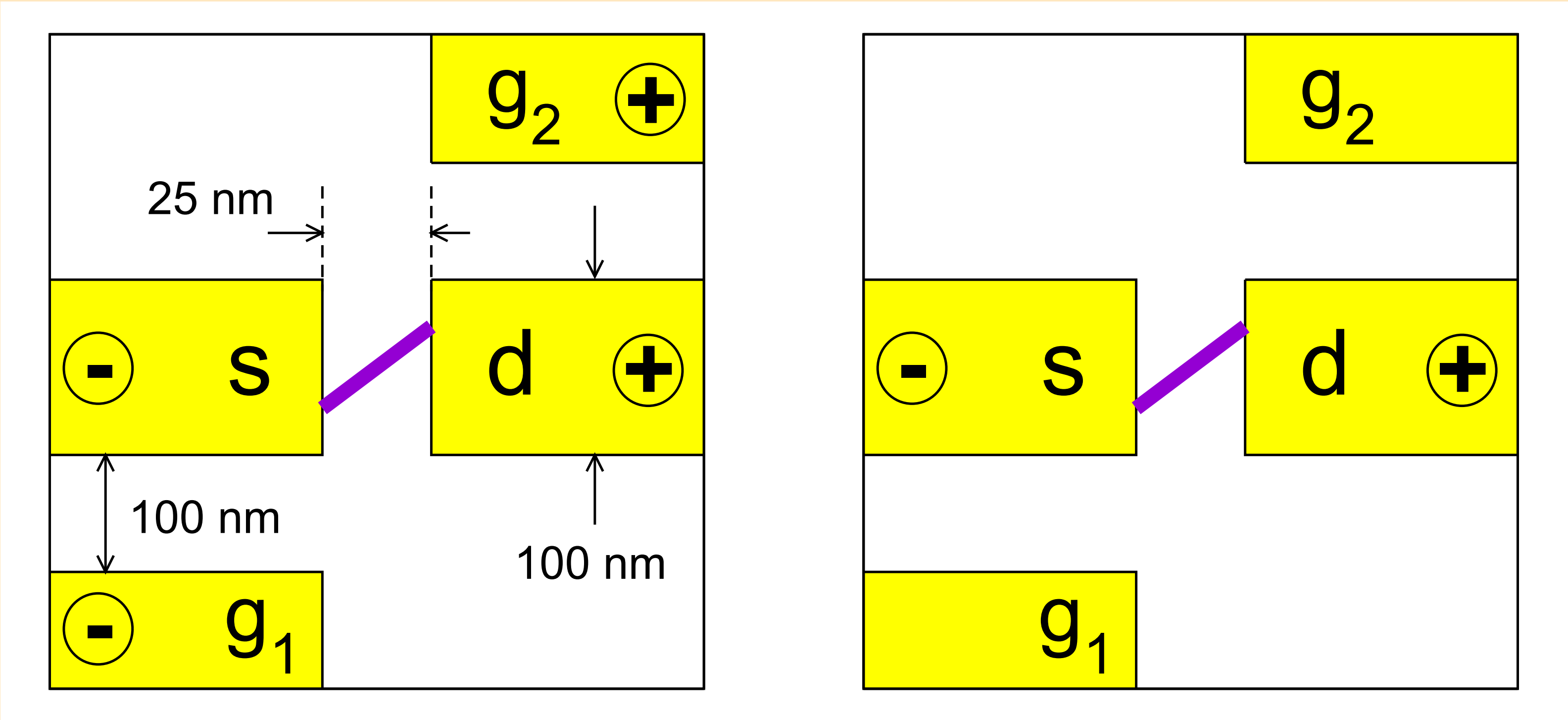


DNA conductivity: experimental set-ups





Proposed experimental set-ups



Trapping:

$V_{sd} \sim 2V$, $V_{g_1 g_2} \sim 30V$

$\alpha \sim 45°$

Measurement:

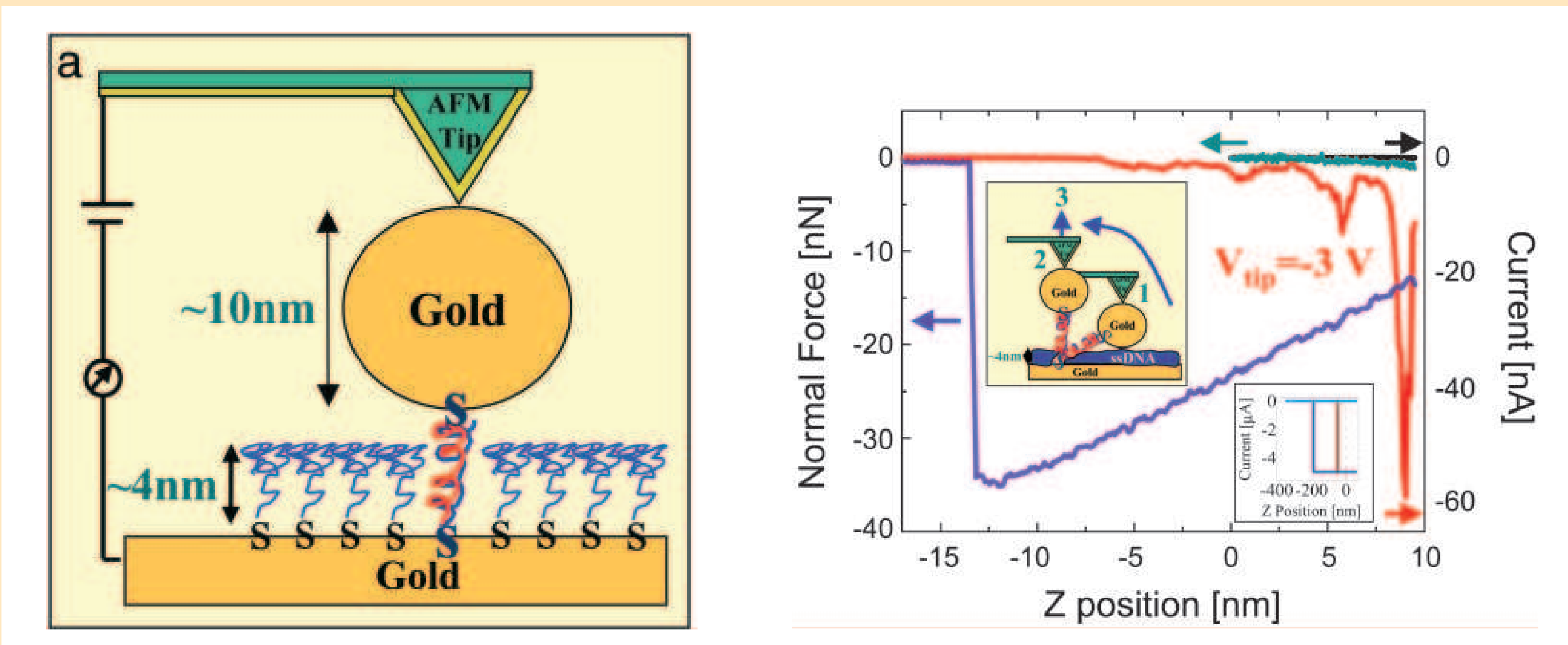
$V_{sd} \sim 2V$

DNA conductivity: experimental set-ups

Direct measurement of electrical transport through single DNA molecules of complex sequence

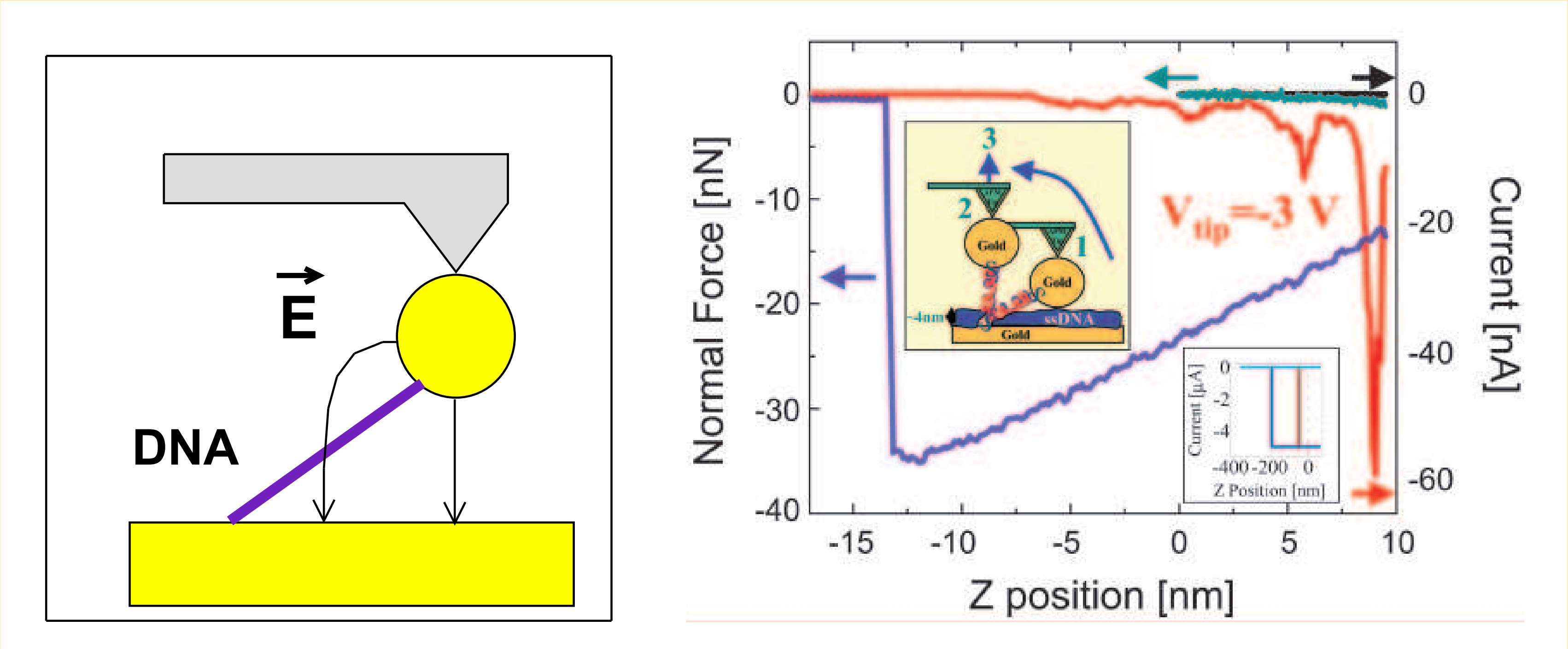
Hezy Cohen*†, Claude Nogues*†‡, Ron Naaman‡, and Danny Porath*§

*Physical Chemistry Department, Hebrew University, Jerusalem 91904, Israel; and ‡Department of Chemical Physics, The Weizmann Institute of Science, Rehovot 7



H. Cohen, C. Nogues, R. Naaman, D. Porath, Proc. Natl. Acad. Sci. **102**, 11589, 2005

Proposed experimental set-ups



Conclusions

- The intrinsic helix conformation of DNA strands determines electric transport properties of the gated double-stranded DNA.

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- The intrinsic helix conformation of DNA strands determines electric transport properties of the gated double-stranded DNA.

- Synthetic semiconducting DNA reveals strong gating effect, which implies various single molecule device applications.

- Tilted periodic DNA sandwiched between two electrodes is a single molecule analog of the Esaki diode

Outlook

- Two experimental set-ups to observe the predicted effect can be proposed:

- A tilted DNA molecule electrostatically trapped between two contacts

- A DNA molecule tiled between the substrate and a nanoparticle suspended from an AFM tip

- Similar argumentation applies also to other helical systems, e. g., the G4-DNA or posiibly proteins.