Bogoliubov Laboratory of Theoretical Physics
Joint Institute for Nuclear Research

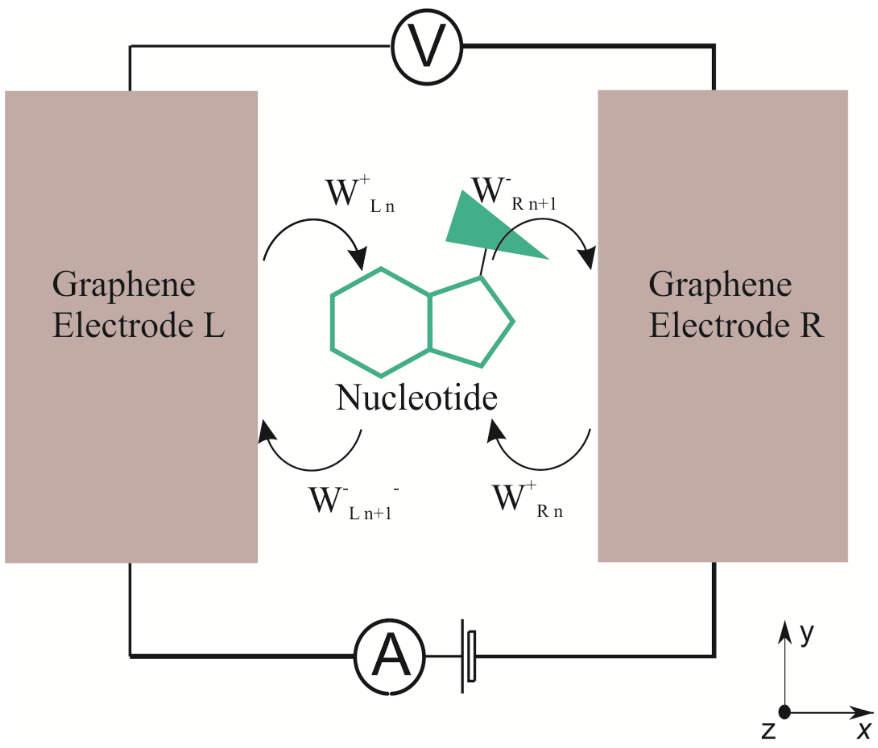
Electron transport through graphene-DNA-graphene junction. DNA decoding

O.G. Isaeva, V.L. Katkov, V.A. Osipov

BRAZIL-JINR FORUM

Dubna June 15-19 2015

Molecular electronic circuit

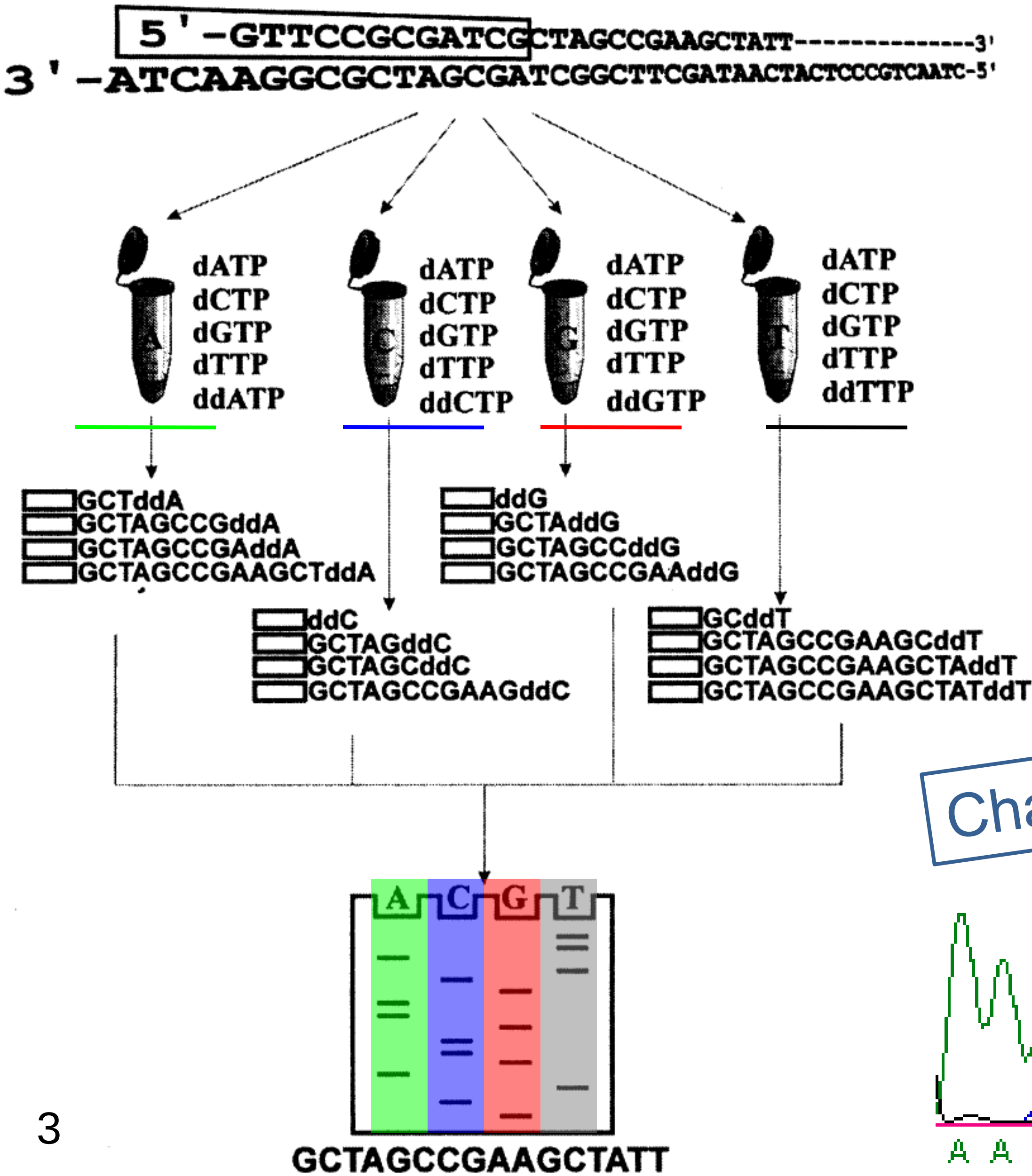


- rectifiers
- transistors
- sensors

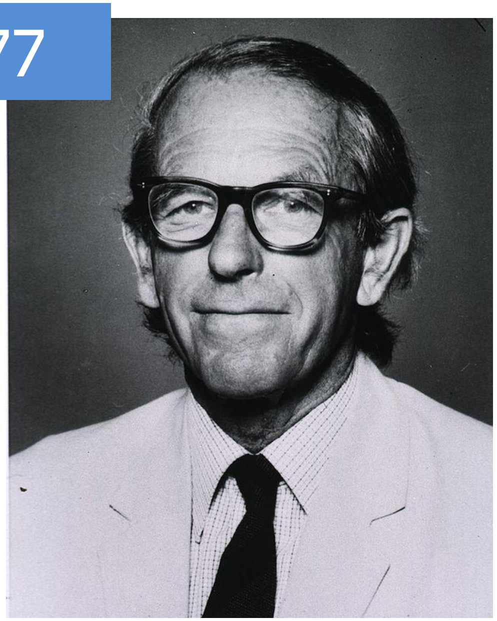
Aviram A. and Ratner M.A. Chem.Phys.Lett. 29 277 (1974)

Sanger method

chemical elongation, electrophoresis

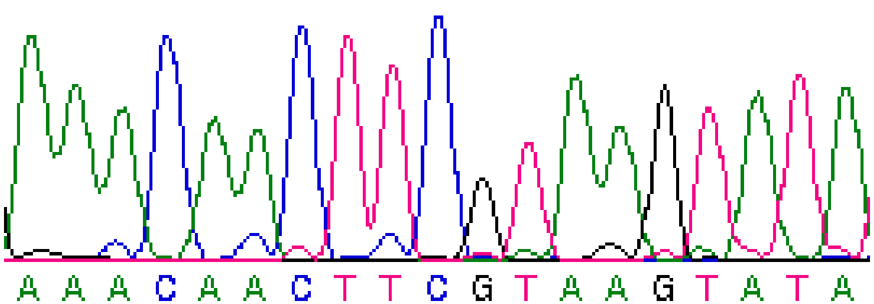


1977



Frederick Sanger
1918-2013

Chain-terminating method



?

- cost of about 10 million USD;
- several months time;

Read-length

human genome

New trends in sequencing methods

(in development):

- effective;
- rapid;
- low-cost

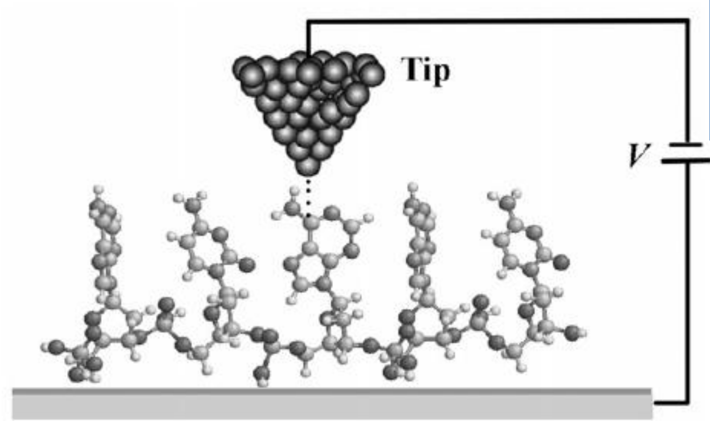
Nanopore concept;

J. Kasianowiez et al., Proc. Natl. Acad. Sci. USA **93** (1996)

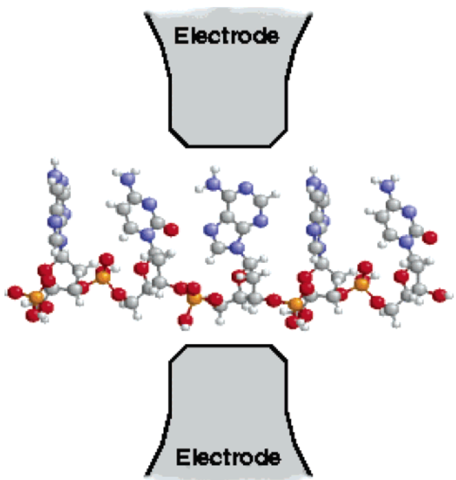
Transverse electronic current;

Zwolak M. and Di Ventra M. Nano Lett. **5** 421 (2005)

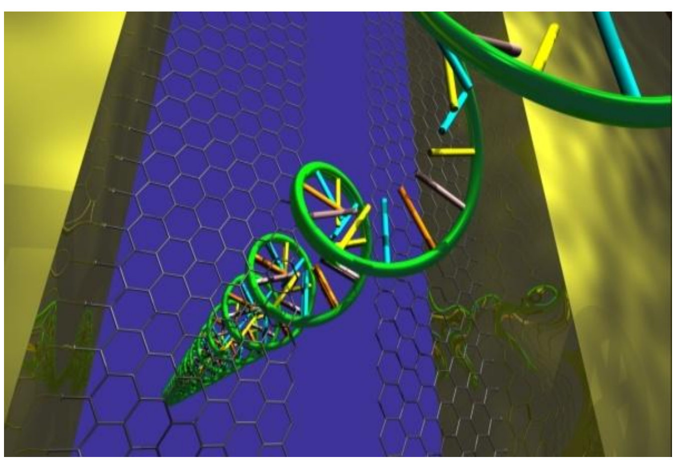
Transverse current for DNA decoding (physical approach)



M.S. Xu et al. Perspectives from Physics, Chemistry and Biology, 2007



Zwolak M. and Di Ventra M. Nano Lett. 5 421 (2005)



H.W.C. Postma NanoLett. 10, 420 (2010)
Prasongkit J. et al NanoLett. 11, 1941 (2011)

L.A. Agapito, J. Gayles, Ch. Wolowiec and N. Kioussis. Nanotechnology, 23 135202 (2012)

Our study

1.The effect of band structure of graphene electrodes (mono, AA, AB) on the on transport properties

V.L. Katkov, O.G. Isaeva, and V.A. Osipov, J. Phys.: Conf. Ser. 393 012026 (2012)

2. The role of both the Coulomb blockade and random positions of nucleotides in the gap for DNA decoding.

*O.G. Isaeva, V. L. Katkov, V. A. Osipov, **DNA sequencing through graphene nanogap: a model of sequential electron transport**, The European Physical Journal B **87**, 272 (2014)*

RESONANT TUNNELING MODEL

$$I = \frac{2e}{h}\int_{-\infty}^{+\infty}\frac{\Gamma_L(\varepsilon-\varepsilon_r-V/2)\Gamma_R(\varepsilon-\varepsilon_r+V/2)}{(\varepsilon-\varepsilon_r)^2-(\Gamma(\varepsilon)/2)^2}\left(f_L(\varepsilon)-f_R(\varepsilon)\right)d\varepsilon$$

$$\Gamma(\varepsilon)=\Gamma_L(\varepsilon-\varepsilon_r-V/2)+\Gamma_R(\varepsilon-\varepsilon_r-V/2)$$

$$\boxed{\Gamma_{L,R}=\hbar\nu\overline{D}_{L,R}}$$

$$\overline{D}_{L,R}=P(\varepsilon)D_{L,R}$$

Channel density:

$$P(\varepsilon)=\frac{n_{L,R}(\varepsilon)}{N_{L,R}}=\frac{2a_0\Delta p_y(\varepsilon)}{h}$$

a_0 is covalent bond length in graphene

Transmission probability:

$$D_{L,R} = \exp[-\lambda(d - d_0)]$$

$$\lambda=\frac{2\sqrt{2m\varphi}}{\hbar}$$

Attempt frequency:

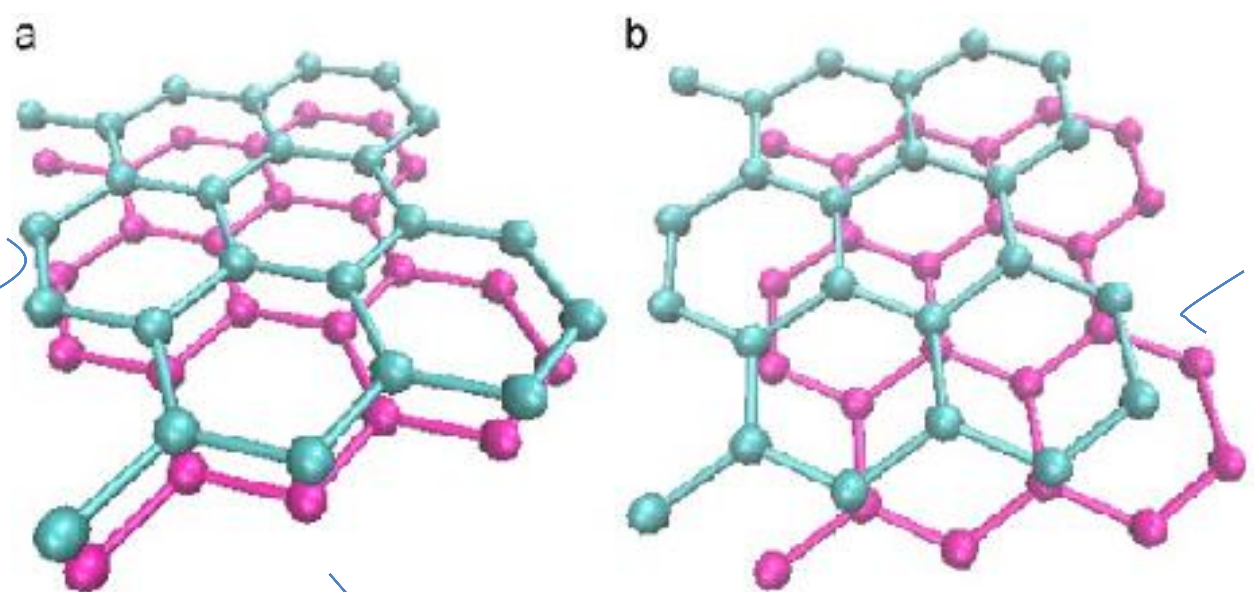
$$\nu=\frac{\hbar}{2md_0^2N}$$

d_0 is covalent bond length in nucleotide

Graphene bilayer

AA bilayer

AB bilayer

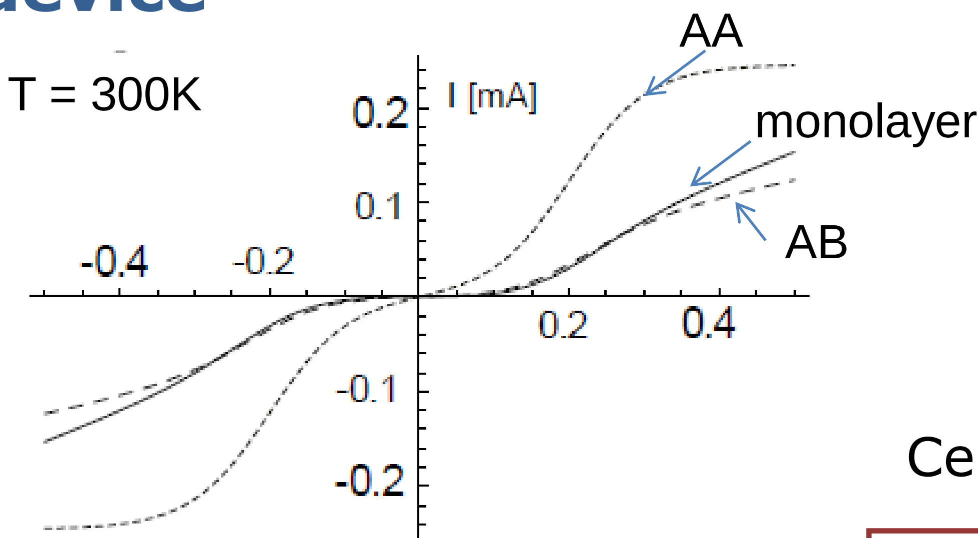


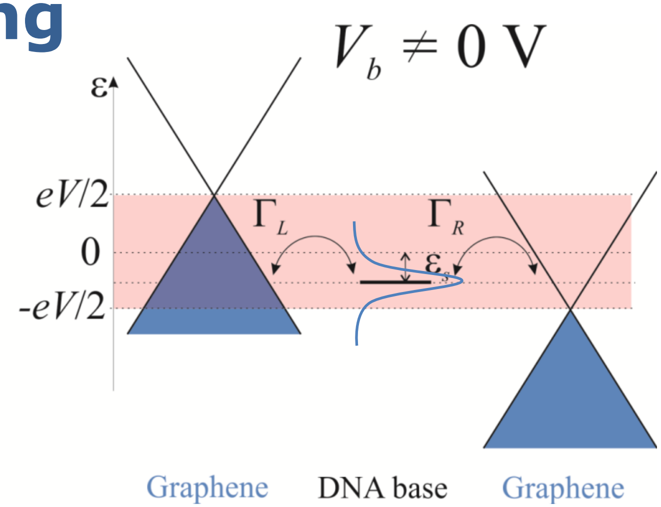
«armchair» edge

«armchair» edge

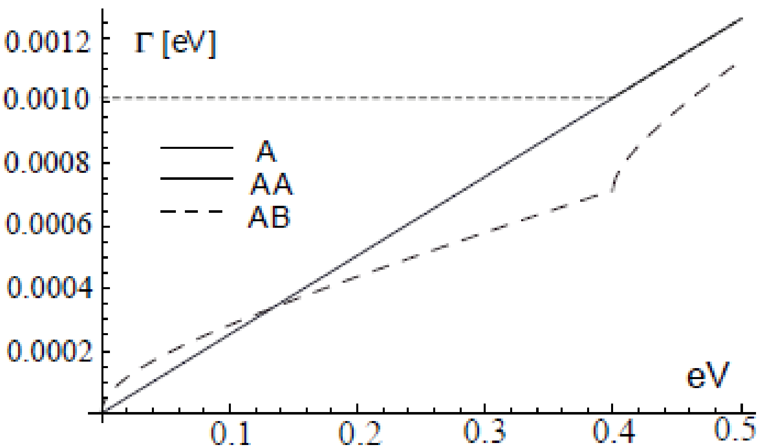
«zig-zag» edge

Results for part one:
I-V characteristics of tunneling device

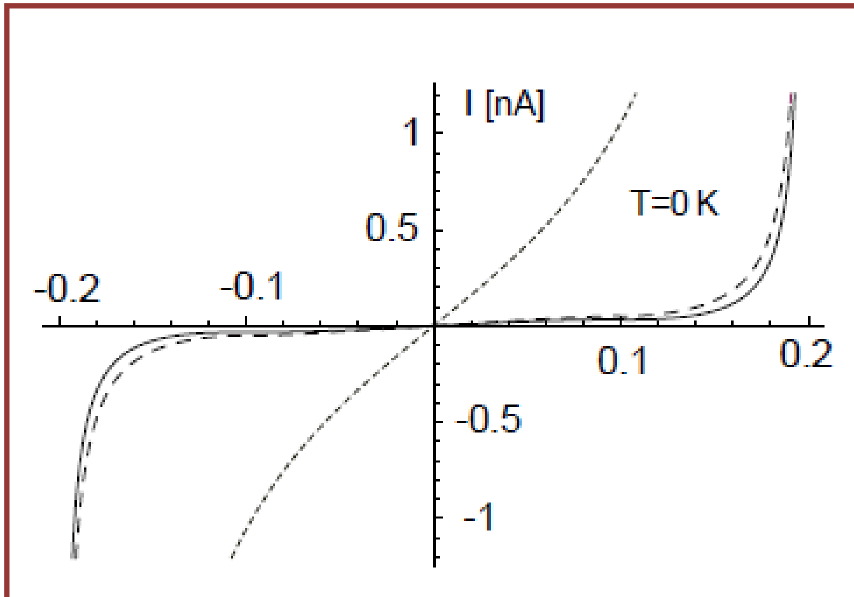




Central part of I-V characteristic



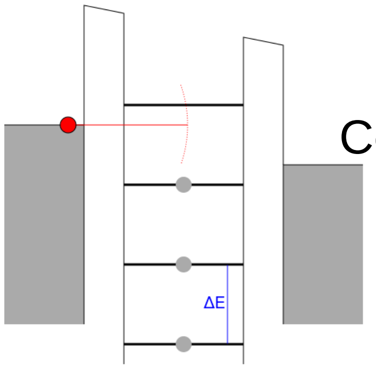
Energy dependence of $\Gamma(\varepsilon)$



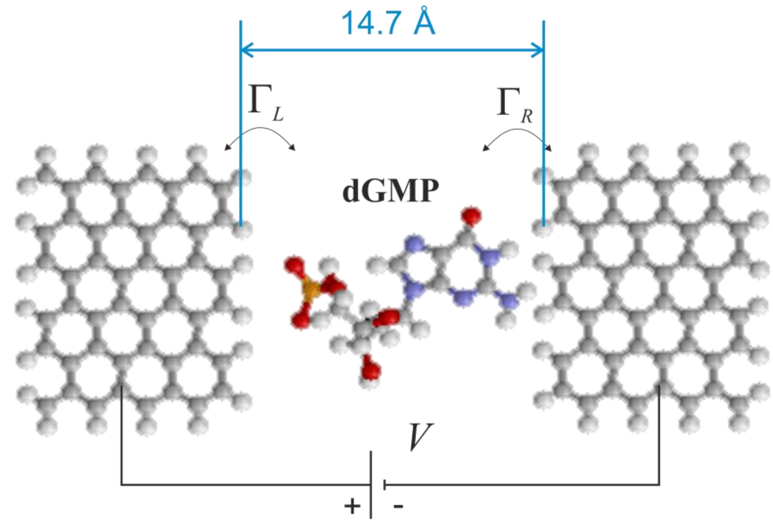
CONCLUSION (for part 1)

Our analysis shows that at the same bias voltage AA graphene bilayer electrodes provide a higher current in comparison with both graphene monolayer and AB bilayer. The use of electrodes on the base of AA graphene bilayer is expected to be much more productive for DNA decoding.

The role of both the Coulomb blockade and random positions of nucleotides in the gap for DNA decoding

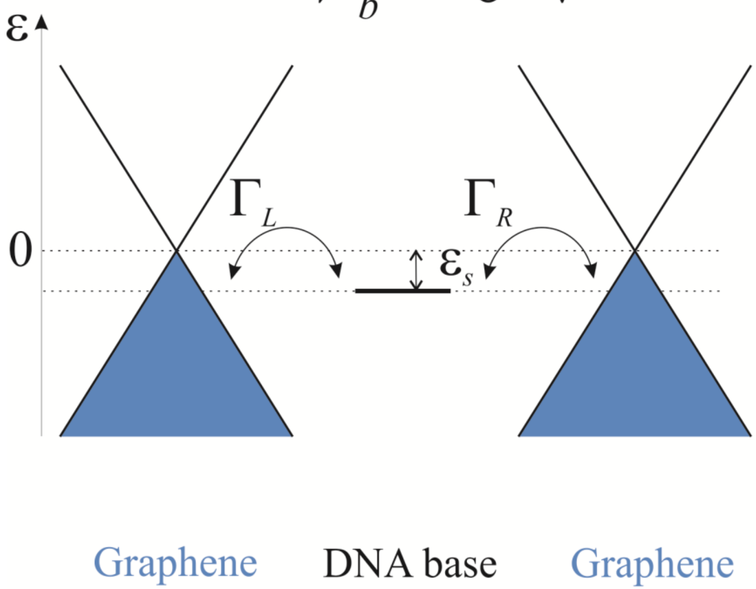


Coulomb blockade

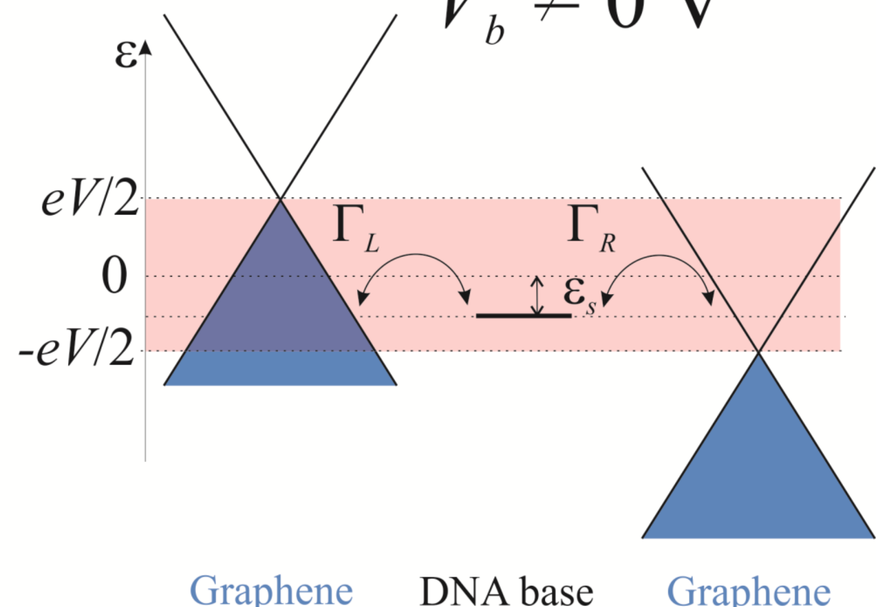


$$\hbar\Gamma_{n\rightarrow n\pm1} << \left|E_n - E_{n\pm1}\right|$$

$V_b = 0$ V



$V_b \neq 0$ V



SEQUENTIAL TUNNELING MODEL

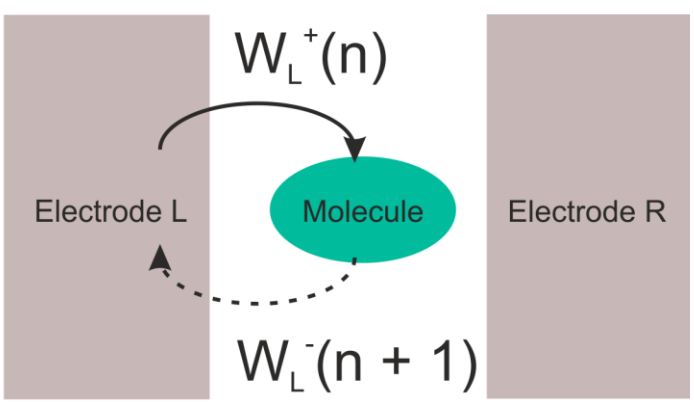
Charge states:

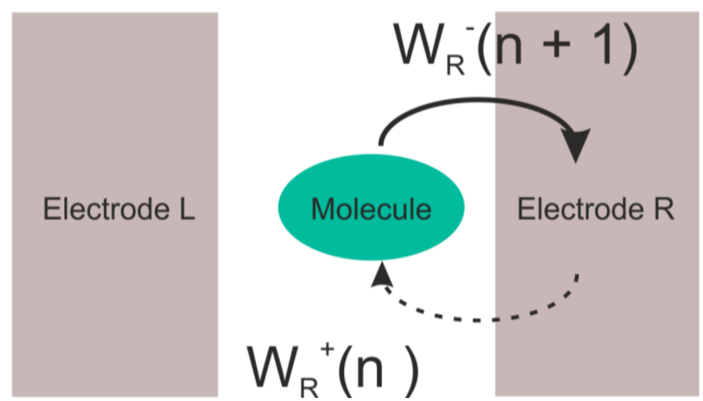
1. n = +2e
   n =+1e
   n = 0e
2. n = +1e
   n = 0e
   n = -1e
3. n = 0
   n = -1e
   n = -2e

Current is calculated by solving a master equation connecting the different charge states *n* = 0 to 2 of the molecule

$$I(V) = \frac{2e}{\hbar} \frac{W_{L0}^{+} W_1^{-} W_2^{-} + W_0^{+} W_2^{-} [W_{L1}^{+} - W_{L1}^{-}] - W_0^{+} W_1^{+} W_{L2}^{-}}{W_1^{-} W_2^{-} + 2W_0^{+} W_2^{-} + W_0^{+} W_1^{+}}$$

$$W_n^{\pm} = W_{Ln}^{\pm} + W_{Rn}^{\pm}$$





D. V. Averin, A. N. Korotkov, and K. K. Likharev, Phys. Rev. B, 44, 6199 (1991)

$$W^{+}_{L(R)}(n) = f(E_{L(R),El\to M})\Gamma_{L(R)};$$

$$W^{-}_{L(R)}(n) = (1 - f(E_{L(R),M\to El}))\Gamma_{L(R)}.$$

$$f(E_{L(R),El\to M}) = \frac{1}{e^{E_{L(R),El\to M}/k_B T} + 1}$$

Elastic tunneling process:

$E_{L(R)\ El\to M} = -\varepsilon_s + U(n+1) - U(n) \mp V/2$

$E_{L(R)\ M\to El} = -\varepsilon_s + U(n) - U(n-1) \mp V/2$

$$U(n) = \frac{n^2 e^2}{2C_{eff}}$$

charging energy of the molecule

Γ_L and Γ_R are tunneling rates.

The Fermi golden rule is used

$$\Gamma_{L,R} = 2\pi \sum_{k_x}\sum_{k_y} \left|T_{L,R}(k_x,k_y)\right|^2 \delta\left(E(k_x,k_y) - \varepsilon\right),$$

$$E(k_x, k_y) = \pm v_F \hbar |\mathbf{k}|$$

Tight-binding approach

$$T_{L,R} = \sum_{i=1}^{N_g} \sum_{j=1}^{N_{A,G,C,T}} C_i^{L(R)} C_j V_{ij}^{L(R)} = \vec{C}^{L(R)} \hat{V}^{L(R)} \vec{C}$$

$V_{ij} = V_{pp\pi} = A\exp[-\beta(d - d_0)]$,

$A = -0.63\dfrac{\hbar^2}{m d_0^2}$, $\beta = 2/d_0$,

L.G.D. Hawke, G. Kalosakas and C. Simserides Eur.Phys.J.E 32, 291 (2010)

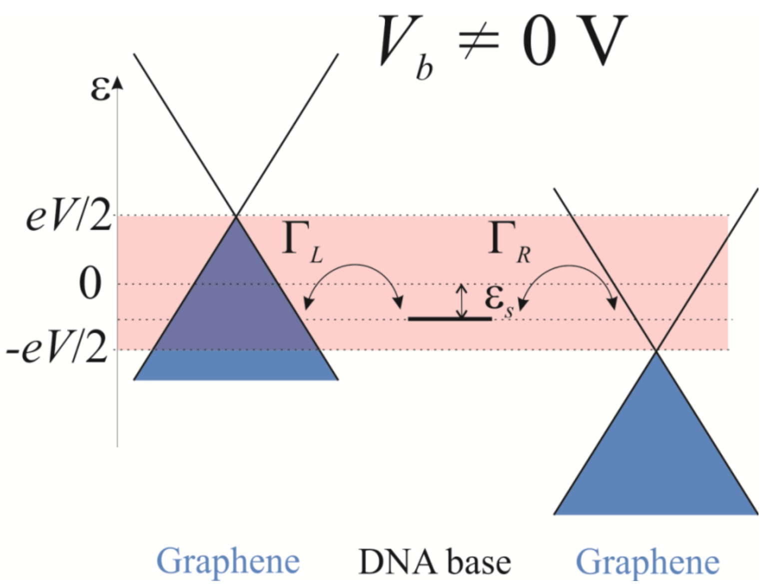
Tunneling rates

$$\Gamma_L(\varepsilon) = \frac{9a_0^2\sqrt{3}}{4\hbar^2 v_F^2}\left[\left(\sum_{i=1}^{i=N_g/2} S_{2i-1}^L\right)^2 + \left(\sum_{i=1}^{i=N_g/2} S_{2i}^L\right)^2\right]|\varepsilon|$$

$$\Gamma_R(\varepsilon) = \frac{9a_0^2\sqrt{3}}{4\hbar^2 v_F^2}\left[\left(\sum_{i=1}^{i=N_g/2} S_{2i-1}^R\right)^2 + \left(\sum_{i=1}^{i=N_g/2} S_{2i}^R\right)^2\right]|\varepsilon|$$

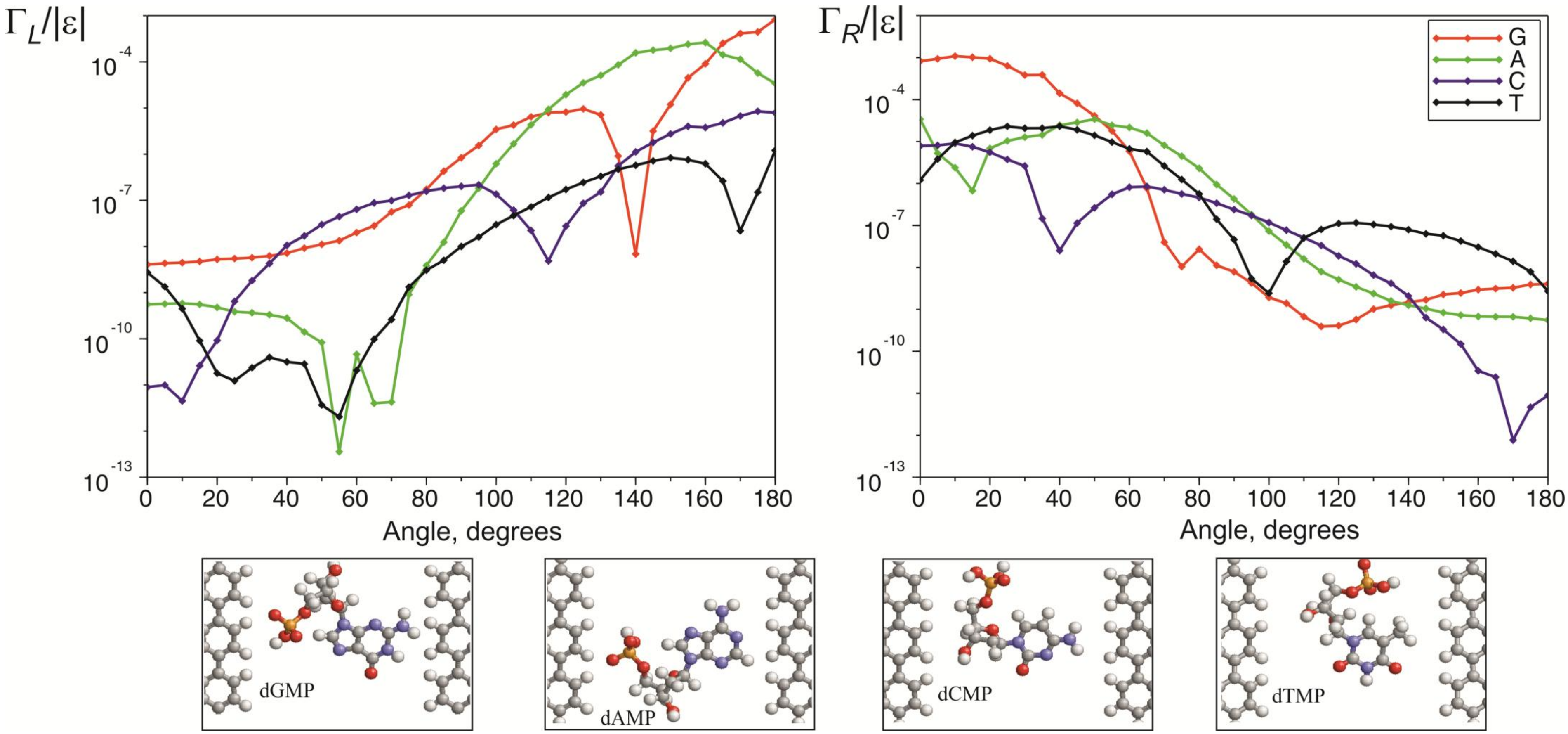
$$\vec{S}^{L(R)} = \hat{V}^{L(R)}\vec{C}$$

$$\varepsilon = -\varepsilon_s + \Delta U(n) \mp V/2$$



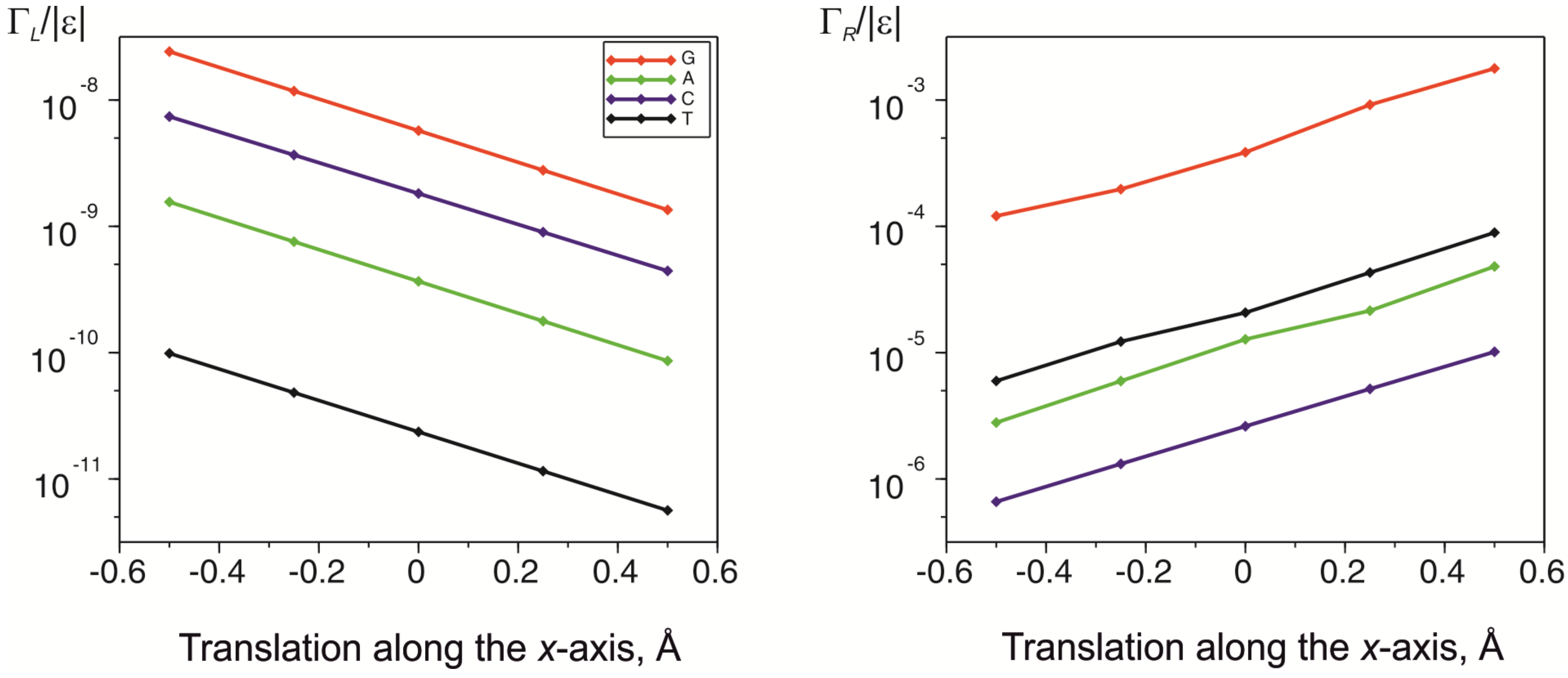
O.G. Isaeva, V. L. Katkov, V. A. Osipov, ***DNA sequencing through graphene nanogap: a model of sequential electron transport****, The European Physical Journal B* ***87****, 272 (2014)*

Results



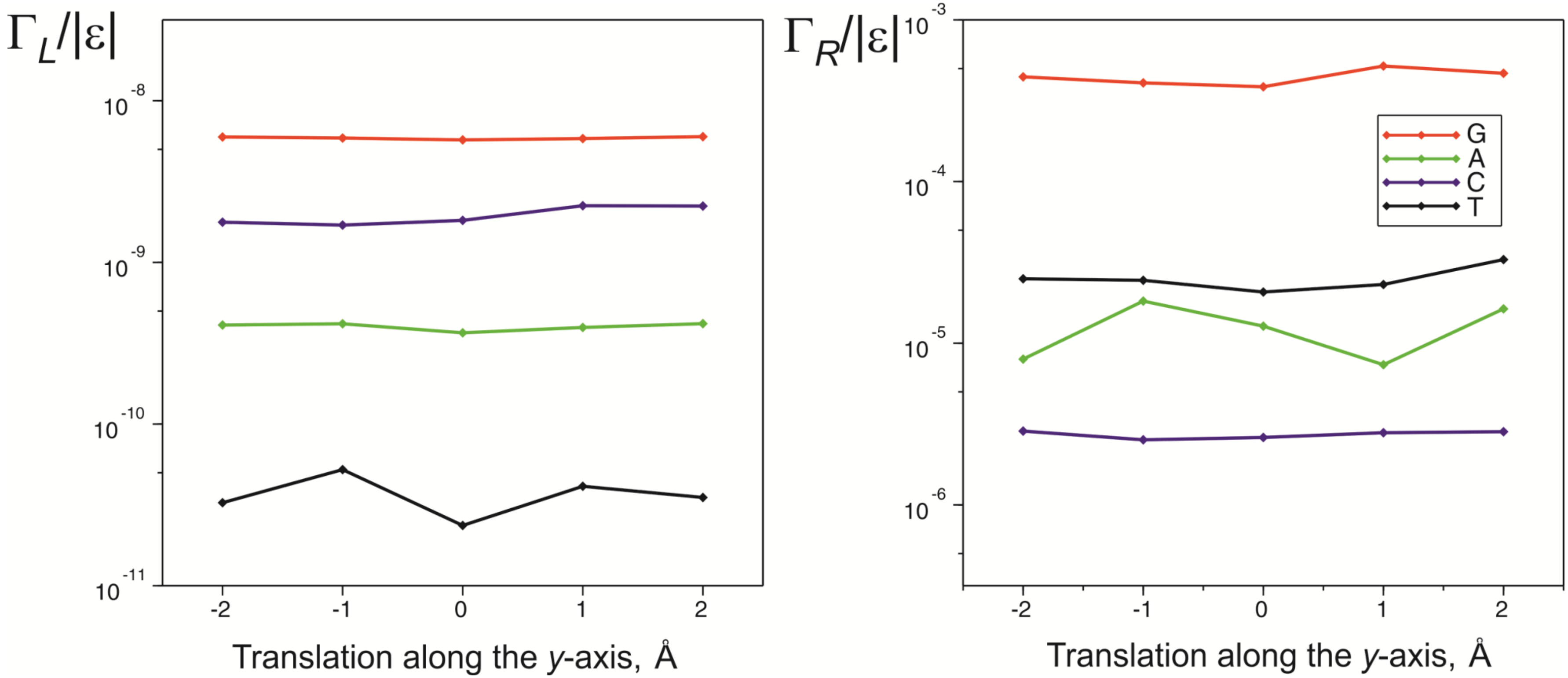
Angular dependences of $\Gamma_L/|\varepsilon|$ (left) и $\Gamma_R/|\varepsilon|$ (right) for dGMP (G), dAMP (A), dCMP (C), and dTMP (T). The pictures below show orientations corresponding to 0°.

Results



$\Gamma_L/|\varepsilon|$ (left) и $\Gamma_R/|\varepsilon|$ (right) as functions of a translation along the *x*-axis. Each nucleotide has fixed angular position 30°

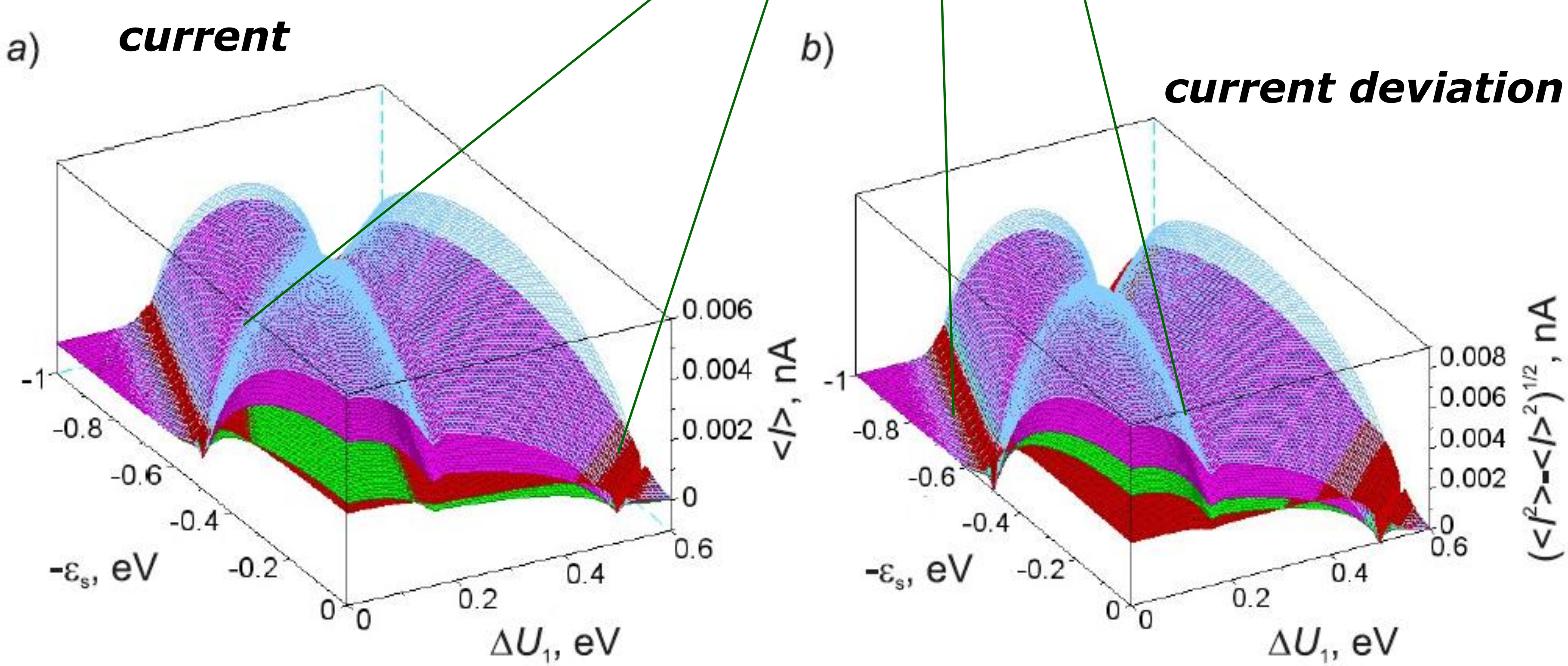
Results



$\Gamma_L/|\varepsilon|$ (left) и $\Gamma_R/|\varepsilon|$ (right) as functions of a translation along the *y*-axis. Each nucleotide has fixed angular position 30°

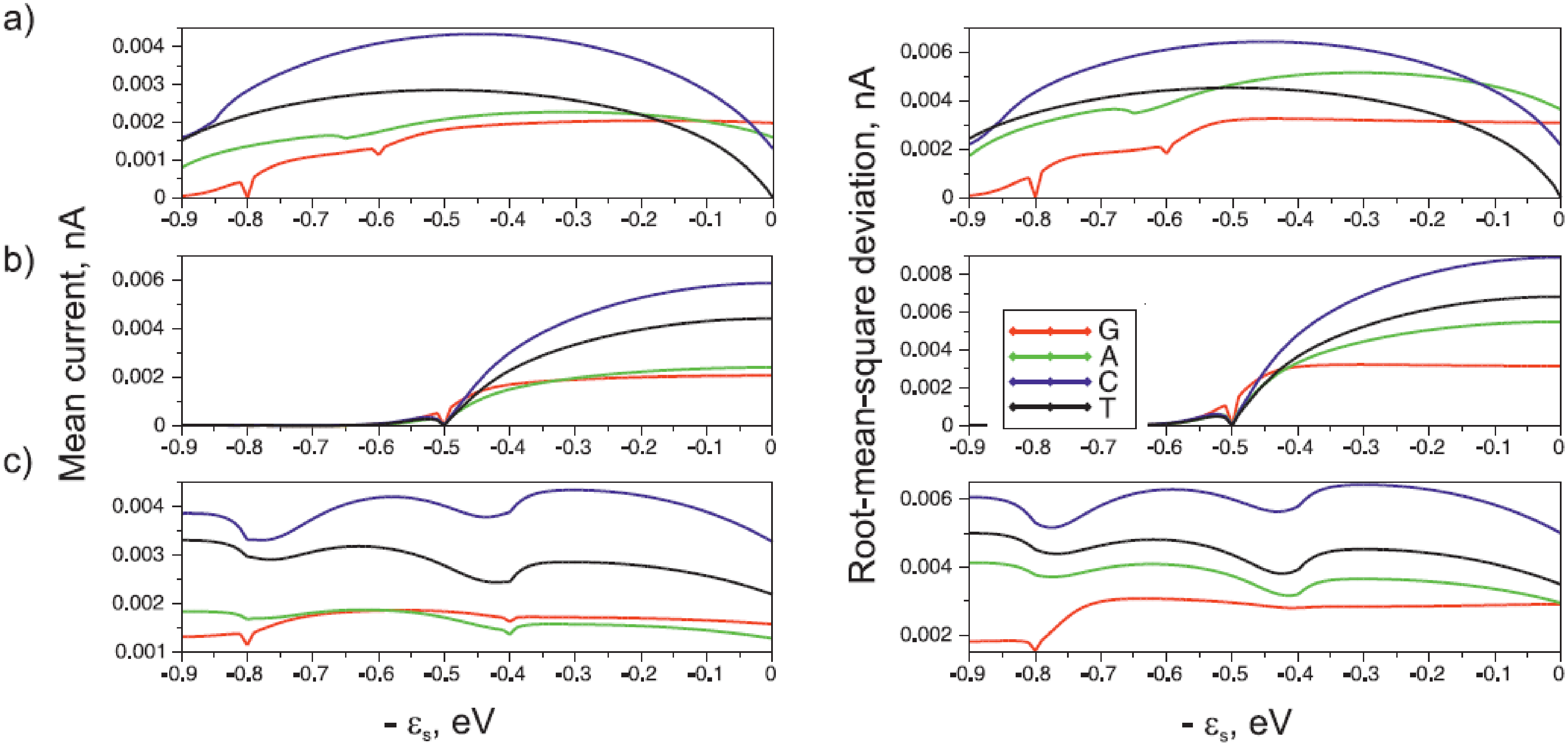
Bias voltage V_b = 1V,
Temperature = 300 K

$$|-\varepsilon_s + U_1| - V_b/2 = 0$$
$$|-\varepsilon_s + 3U_1| - V_b/2 = 0$$



dGMP dAMP dCMP dTMP

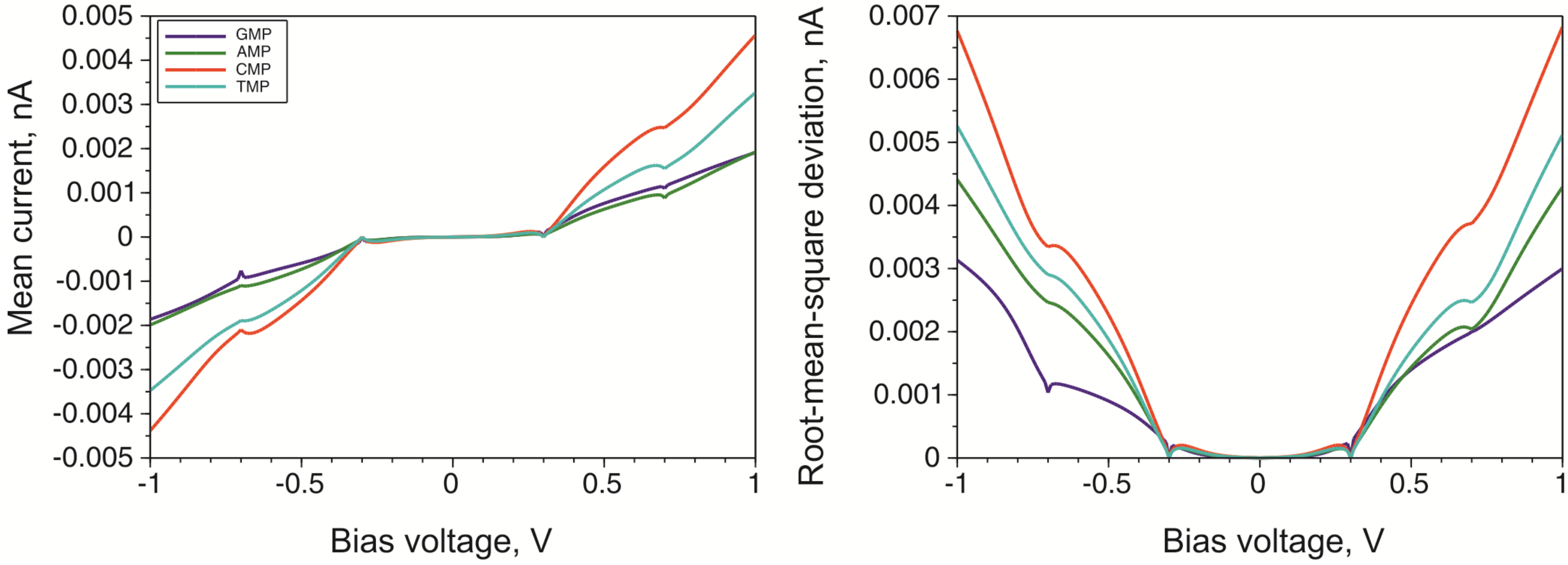
Bias voltage V_b = 1V,
Temperature = 300 K



a) ΔU_{1G} = 0.1 eV, ΔU_{1A} = 0.15 eV, ΔU_{1C} = 0.45 eV, ΔU_{1T} = 0.5 eV;

b) ΔU_1 = 0 eV (for each nucleotide);

c) ΔU_1 = 0.3 eV (for each nucleotide).



Mean I-V characteristics (left). rmsd vs voltage (right). Parameters for calculation: ε_s = -0,4 эВ, ΔU_1 = 0,25 эВ, T = 300 К

CONCLUSION (for part 2)

- Unique shape of each nucleotide provides a specific dispersion of tunnel currents so that combined measurements of the tunnel current and its root-mean-square deviation allow to facilitate the identification of nucleotides

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Thank you for attention

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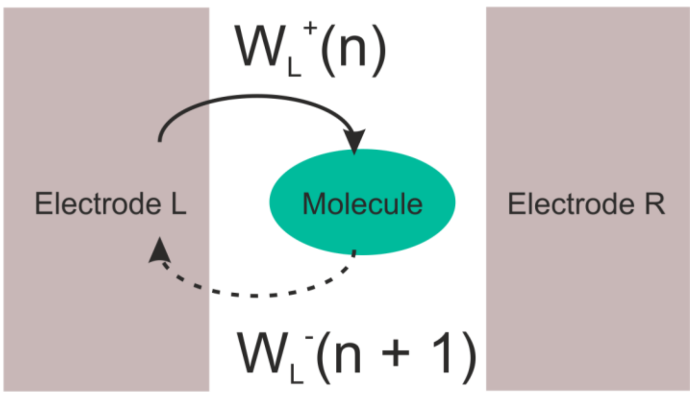
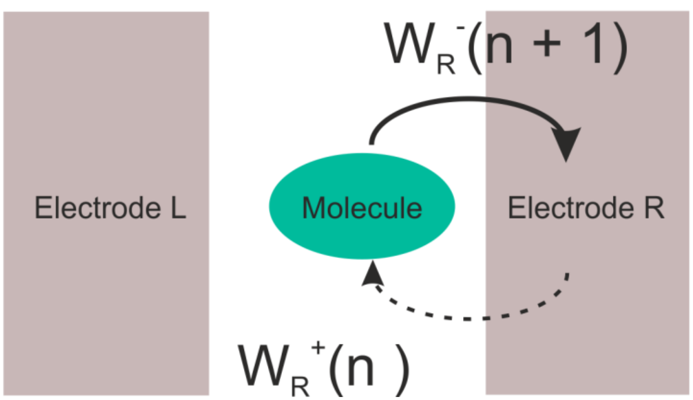
Current is calculated by solving a master equation connecting the different charge states *i* = 0 to 2 of the molecule



$$\frac{d\sigma(n)}{dt} = W^+(n-1)\sigma(n-1) + W^-(n+1)\sigma(n+1) -$$
$$-(W^+(n) + W^-(n))\sigma(n);$$
$$\sum_{i=0}^{2} \sigma(n+i) = 1;$$
$$W^{\pm} = W_L^{\pm} + W_R^{\pm}$$



$$W^-(n+1)\sigma(n+1) = 2W^+(n)\sigma(n);$$
$$2W^-(n+2)\sigma(n+2) = W^+(n+1)\sigma(n+1)$$

$$\boxed{I = -e\sum_{i=0}^{2} \sigma(n+i)(W_L^+(n+i) - W_L^-(n+i))}$$

D. V. Averin, A. N. Korotkov, and K. K. Likharev, Phys. Rev. B, 44, 6199 (1991)