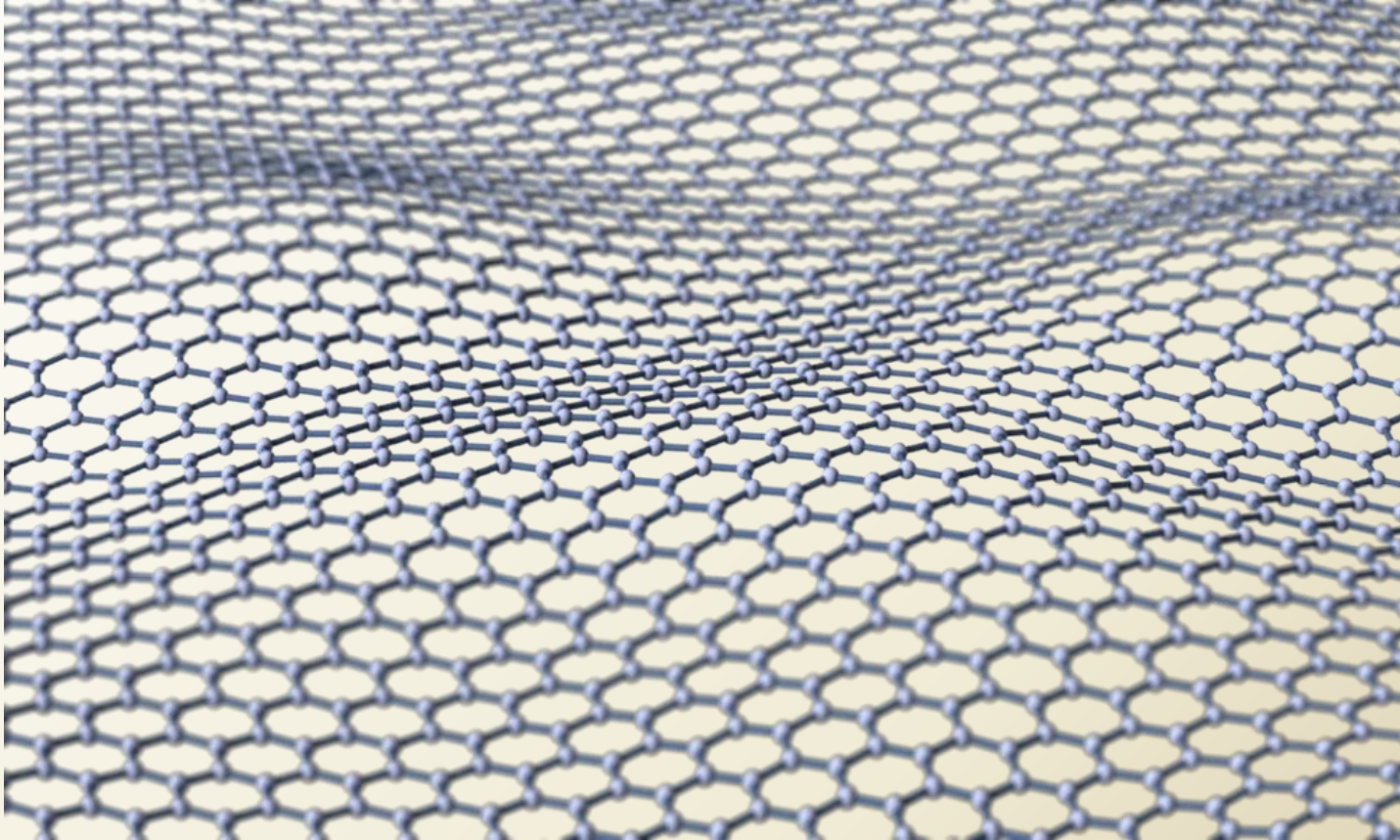


# Graphene-based tunnel junction



Vsevolod Katkov  
BLTP Sector № 16

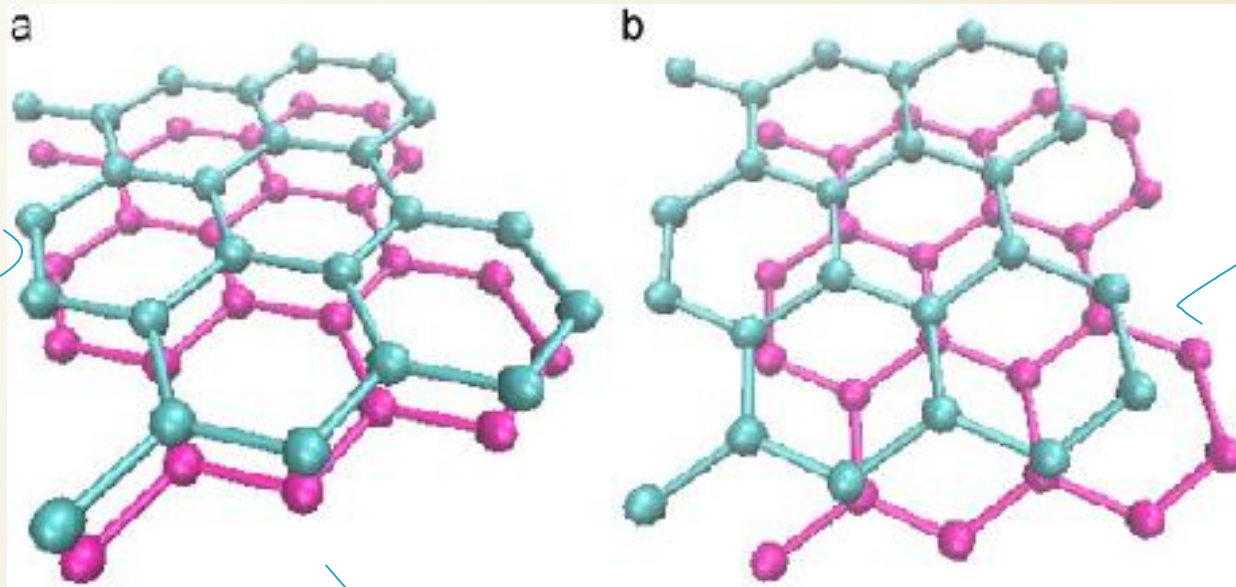
# What is graphene



# What is graphene

AA bilayer

AB bilayer



«armchair»  
edge

«armchair»  
edge

«zig-zag» edge



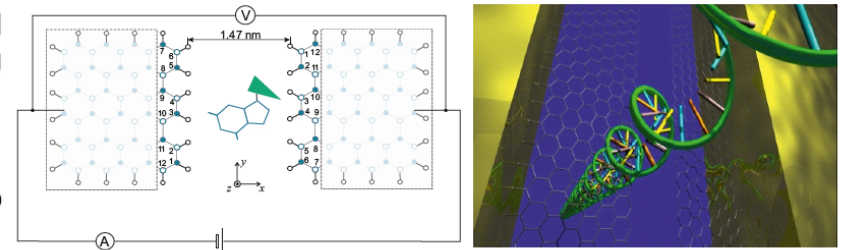
# A model of sequential electron transport in the system graphene-nucleotide-graphene. DNA decoding

O.G. Isaeva, V.L. Katkov and V.A. Osipov (E-mail: issaeva@theor.jinr.ru)

*Bogoliubov Laboratory of Theoretical Physics Joint Institute for Nuclear Research*

Electron transport through nucleotide in graphene nanogap is studied within the sequential tunneling model using the tight-binding approximation and the master equation technique.

Both the Coulomb blockade and random positions of nucleotides: angular orientations and shifts in the electrode plane are taken into account.



*A rapid and low-cost method of DNA decoding*

## Model

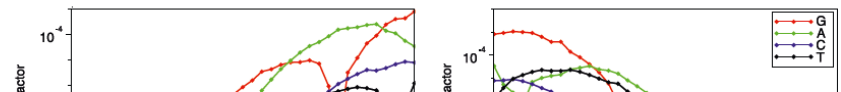
Each nucleotide is assumed to be coupled via tunnel barriers to two electron reservoirs of the electrodes. During the transfer of electron from the electrode to the nucleotide and backwards, subsequent charging and discharging of the molecule occurs. Therefore the nucleotide can take three allowed charge states ( $n = 0, 1, 2$ ) in the process of tunneling. The current in the circuit is calculated by formula:

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

$\vec{S}^{L(R)} = \hat{V}^{L(R)} \vec{C}$  Here  $\vec{C}$  is eigenvector of nucleotide at given energy state,

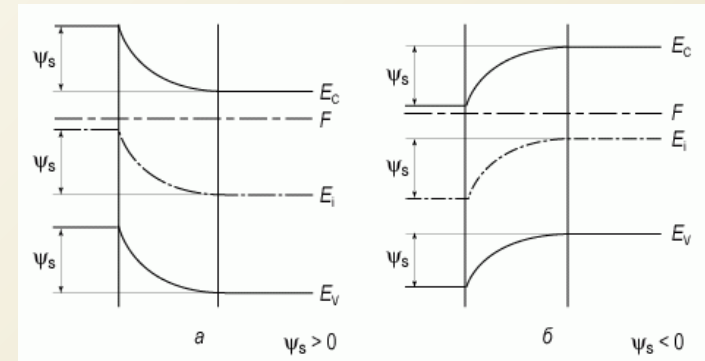
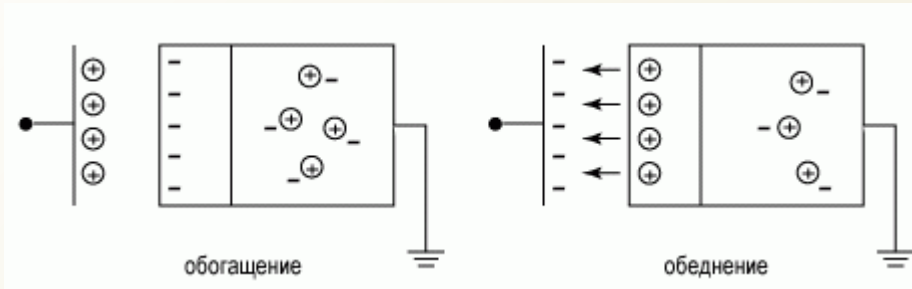
$V_{ij}^{L(R)} = A \exp(-\beta(d_{ij}^{L(R)} - d_0))$  is the hopping parameter [5], where  $d_{ij}^{L(R)}$  is a distance between  $i$ th atom of graphene and  $j$ th atom of nucleotide,  $A = -0.63\hbar^2 / (m_e d_0^2)$ ,  $\beta = 2 / d_0$

## Results and Conclusion

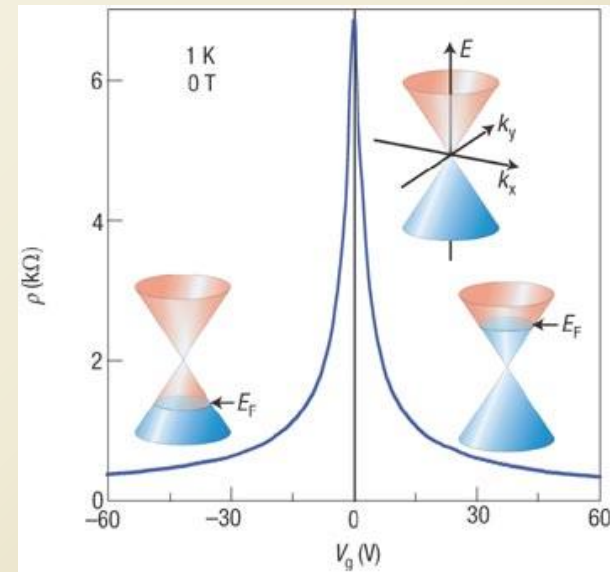
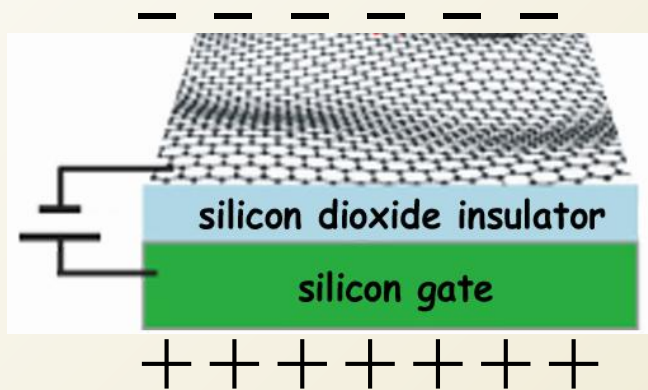


# Graphene under gate

Semiconductor

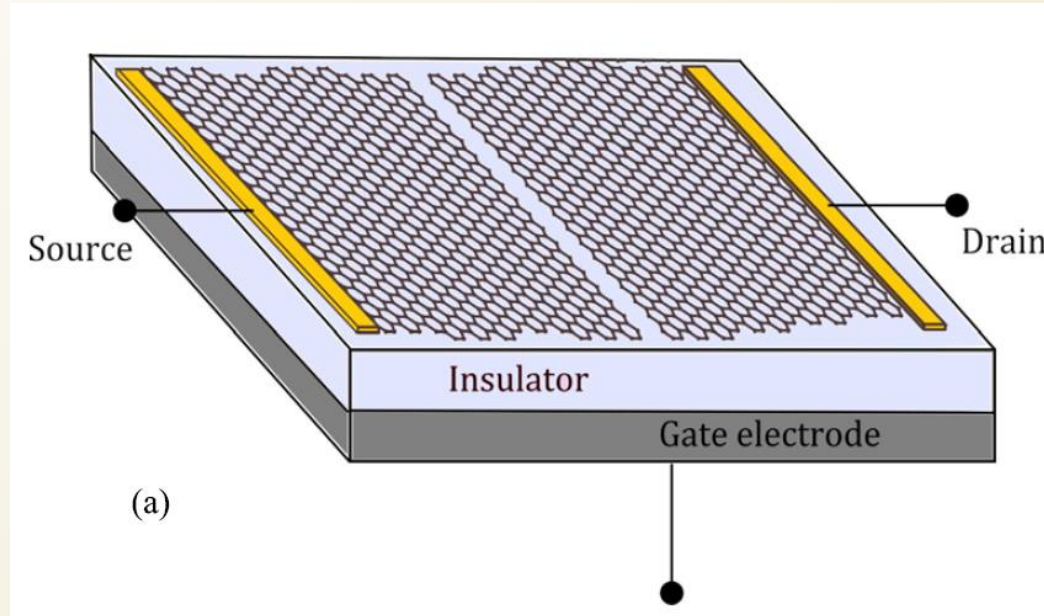


## Graphene



*mobility*  $> 15000 \text{ cm}^2\text{V}^{-1}\text{s}^{-1}$

# Tunnel field-effect transistor (TFET)



Schematic picture of graphene planar TFET

# Quantum transport calculation: The Green's Function approach + tight binding approximation

$$I = \frac{e}{h} \int_{-\infty}^{\infty} \text{Tr}[A_L(\mathbf{1} - t^\dagger g_R^- t g_L^-)^{-1} t^\dagger A_R t (\mathbf{1} - g_L^+ t^\dagger g_R^+ t)^{-1}] [f_L - f_R] d\varepsilon,$$

$g_{R,L}^\pm = [(\varepsilon + i0^+) \mathbf{1} - H_{R,L}]^{-1}$  - calculated numerically by Sancho-Rubio fast iterative technique

$$A_{R,L} = i(g_{R,L}^+ - g_{R,L}^-)$$

is the spectral density

$$t = \sum_{i,j} t_m^{ij} c_{L,i}^\dagger c_{R,j}$$

M.P. Lopez Sancho, J.M. Lopez Sancho and J. Rubio, Phys. F: Met. Phys. **14**, 1205 (1984)

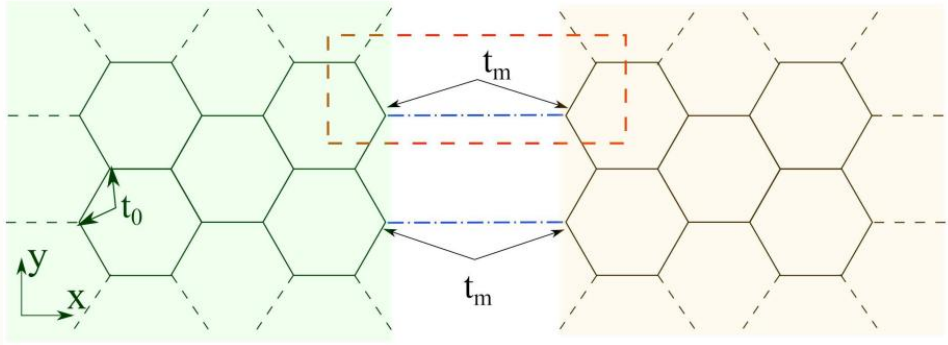
M.P. Lopez Sancho, J.M. Lopez Sancho and J. Rubio, Phys. F: Met. Phys. **15**, 851 (1985)

$$\rho_l^n = -\text{Im}(g_{nn})/\pi.$$

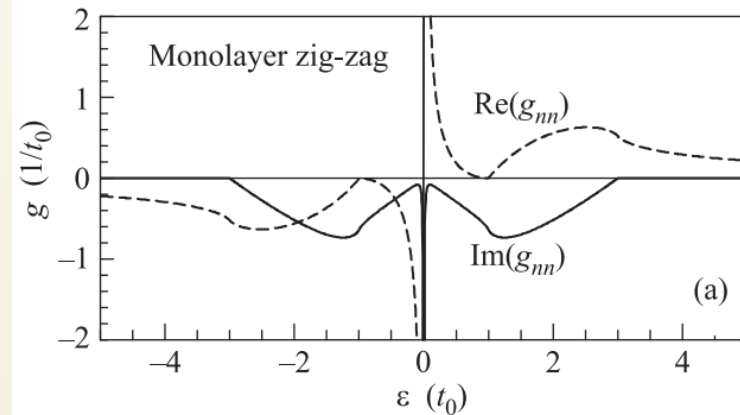
The local density of electronic states for the  $n$  th atom

T = 300 K

$$H_{L,R} = (\pm eV/2 + eV_g) \sum_i c_{(L,R),i}^\dagger c_{(L,R),i} + t_{ij} \sum_{i,j} c_{(L,R),i}^\dagger c_{(L,R),j},$$

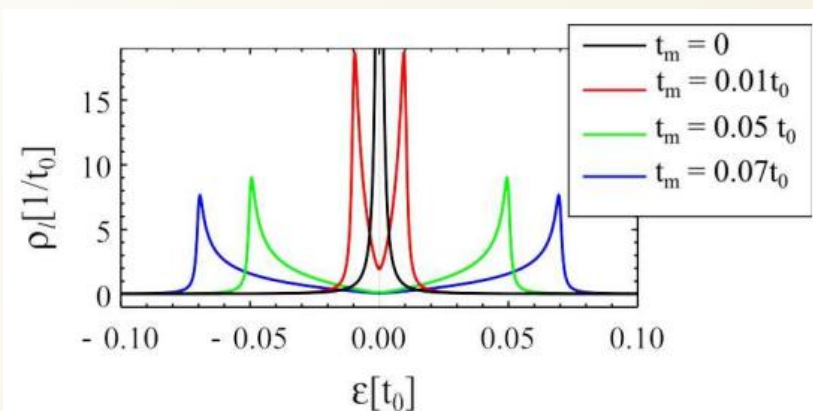


Atomic structure of a junction.

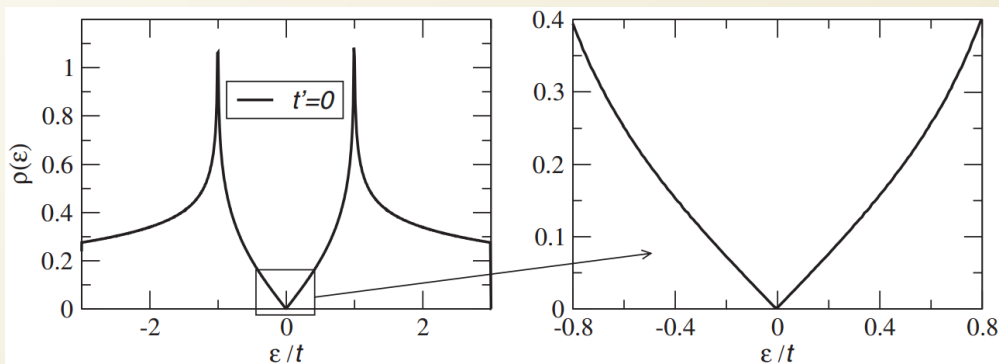


The Green's function for the contacting atoms

$$\rho_l^n = -\text{Im}(g_{nn})/\pi.$$

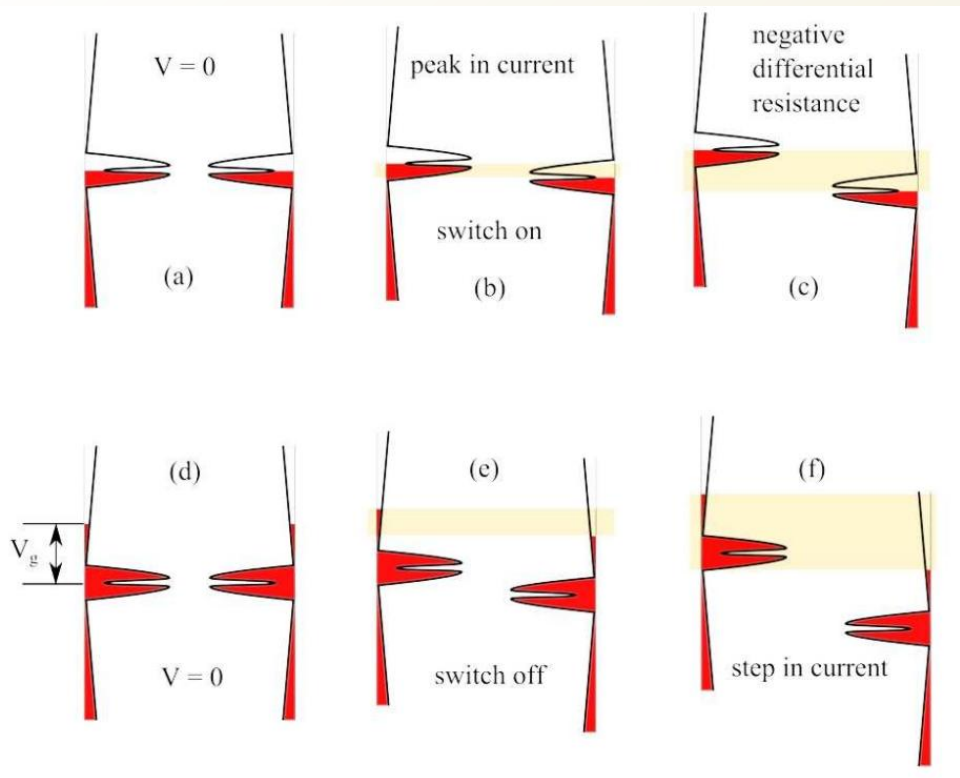


Local DOS of edge atoms at different interaction constants between tunnel contacts.

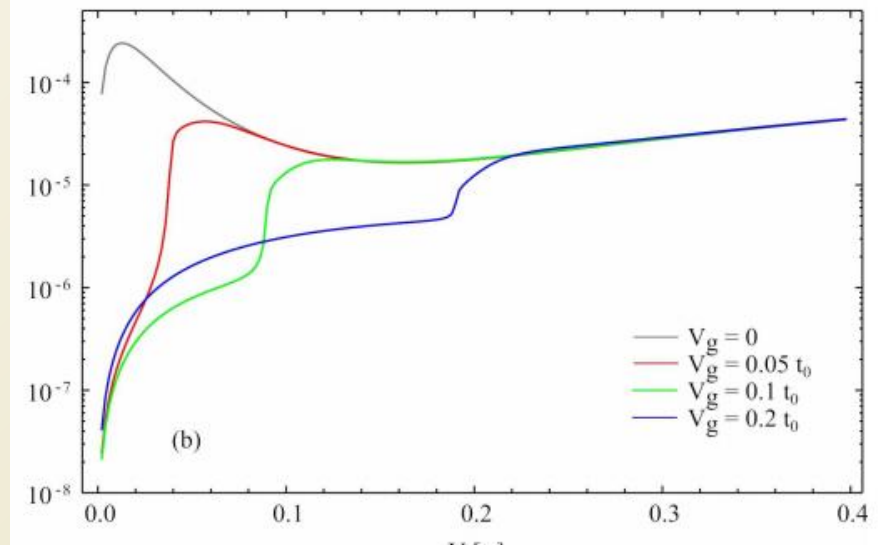
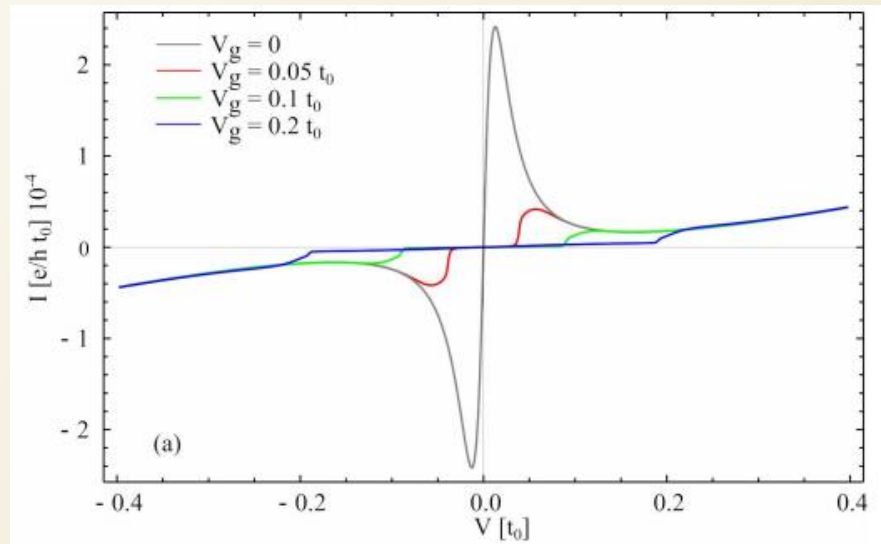


DOS for bulk graphene from  
*The electronic properties of graphene*  
 Rev. Mod. Phys. **81**, 109 (2009)  
 H. Castro Neto, F. Guinea,  
 N. M. R. Peres, K. S. Novoselov, and A. K. Geim

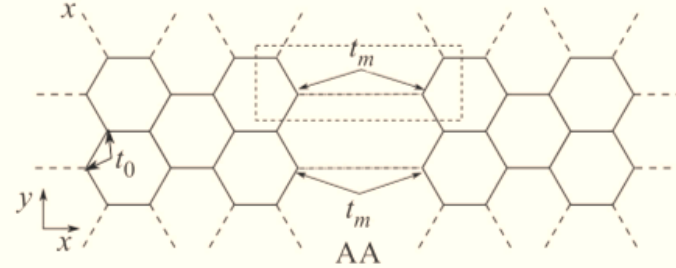
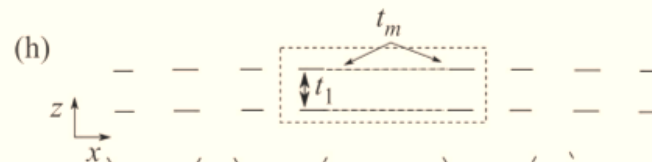
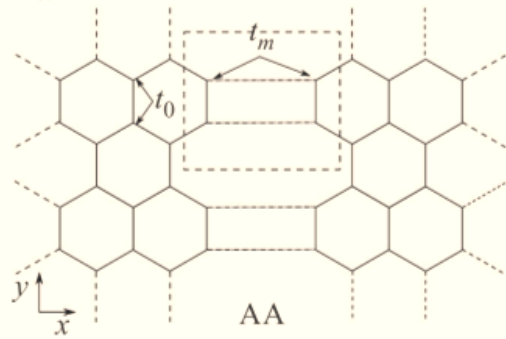
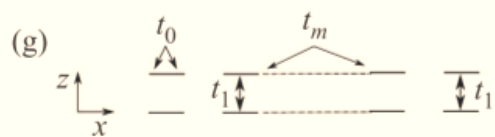
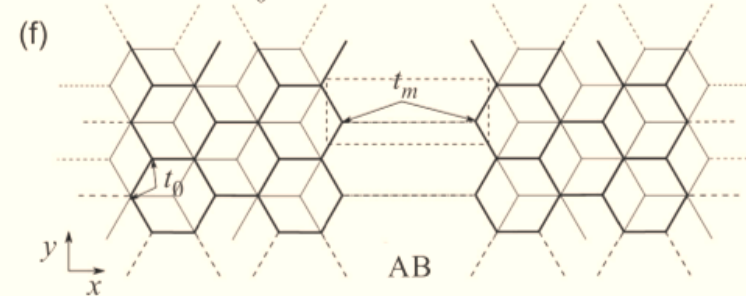
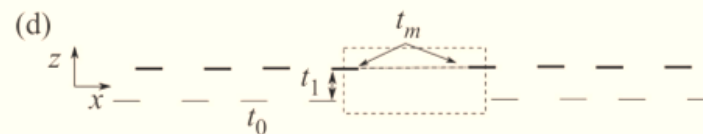
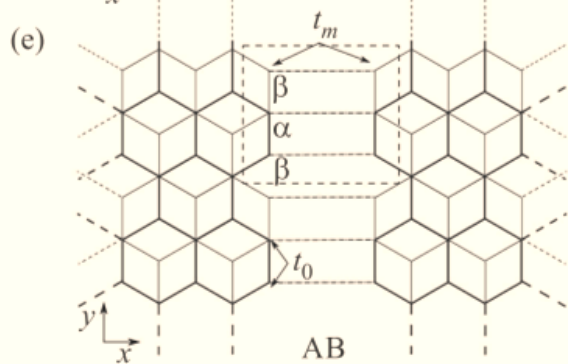
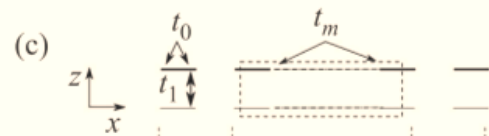
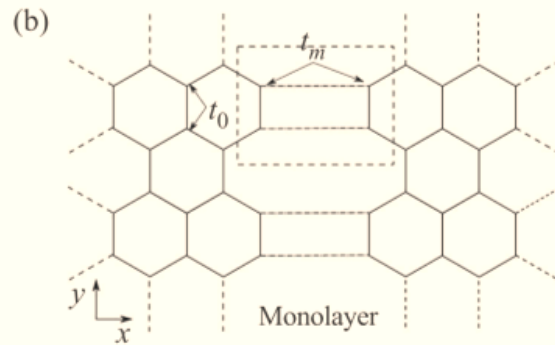
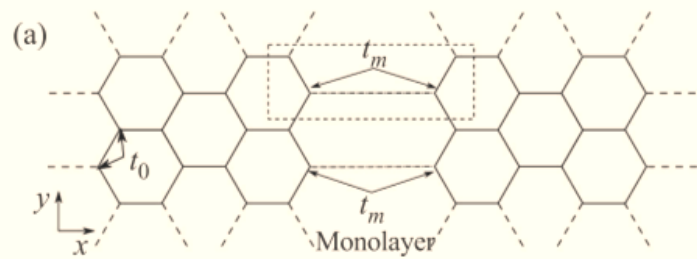




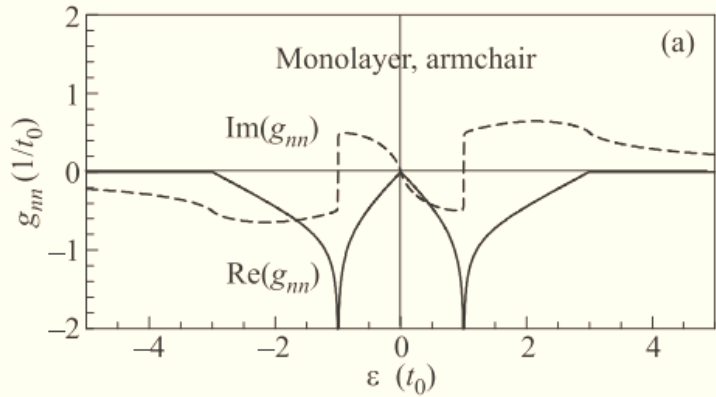
Schematic electronic DOS diagram. The filled states have a red color. Yellow region shows the energy window: carriers can now tunnel into empty states in the right contact.



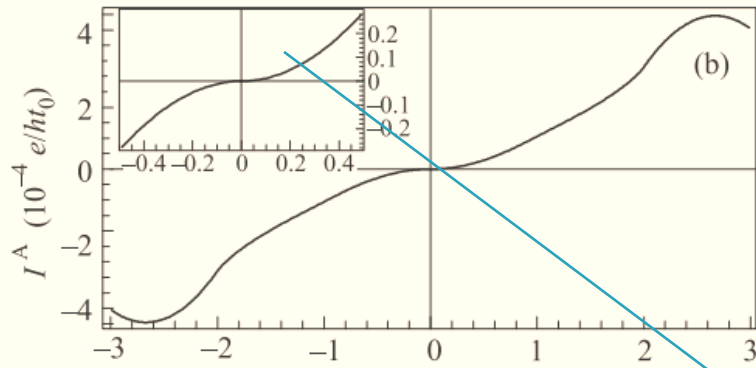
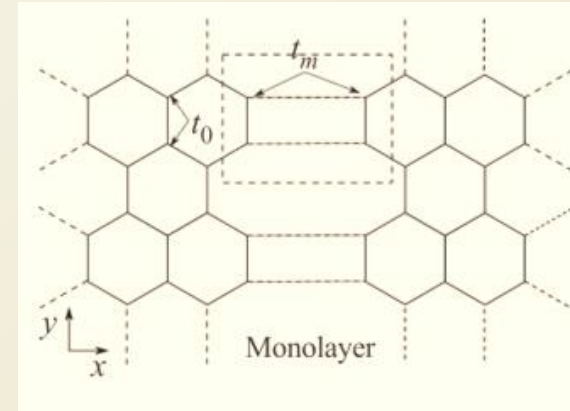
I-V characteristics of graphene TFET at different gate voltages



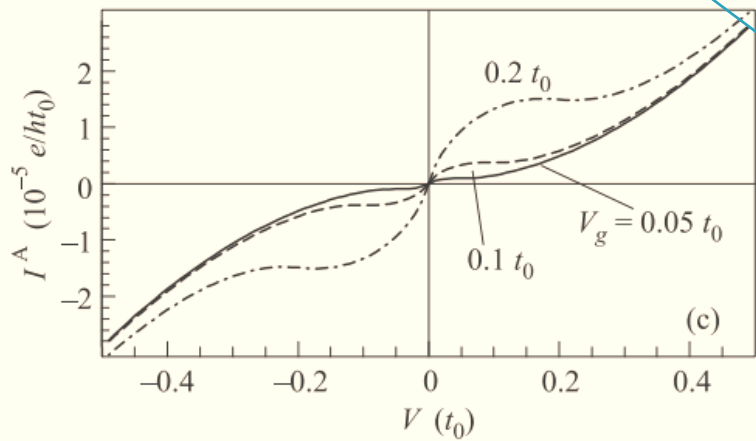
# monolayer, armchair



Green's function  
for the contacting atoms



current-voltage curve

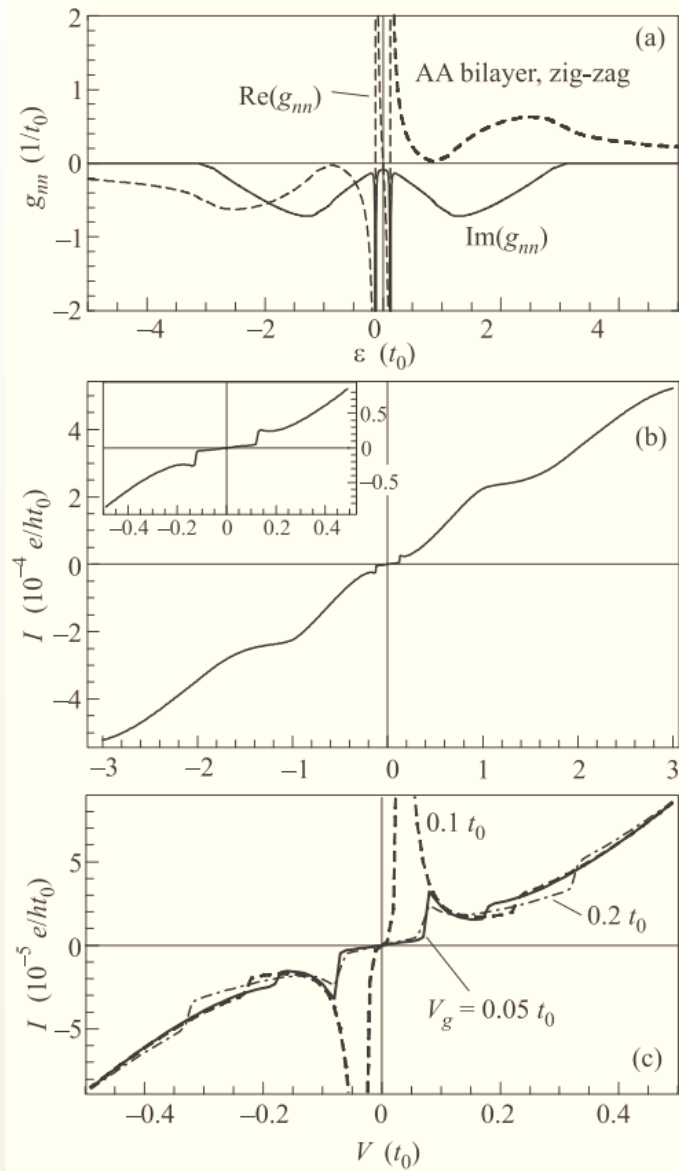


The transfer Hamiltonian approach gives:

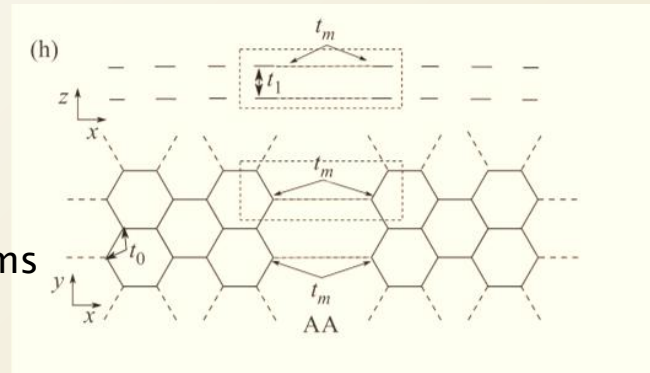
$$I^A \simeq 1.18 \text{sign}(V) \frac{e}{h} \frac{t_m^2}{t_0^3} V^2$$

current-voltage curve for the  
gate voltage  $V_g = 0.05t_0$ ,  $0.1t_0$ , and  $0.2t_0$

# AA bilayer, zigzag



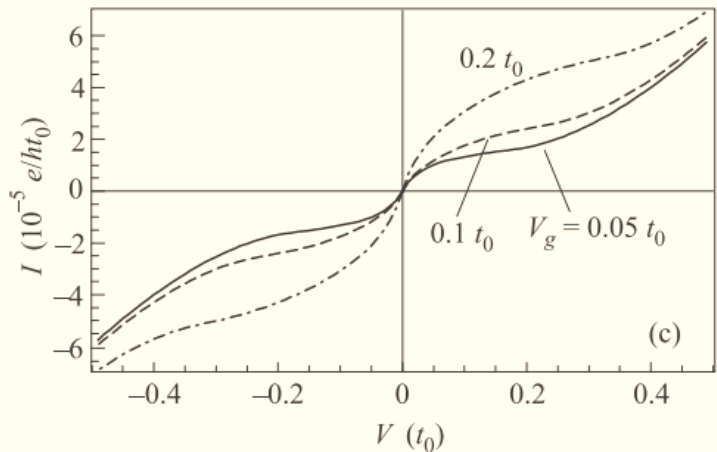
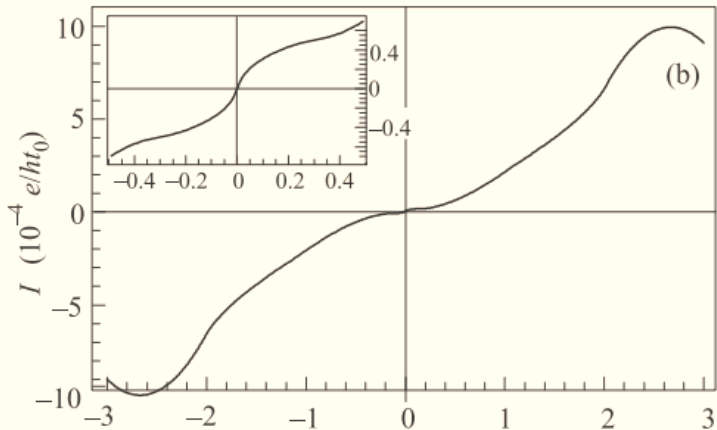
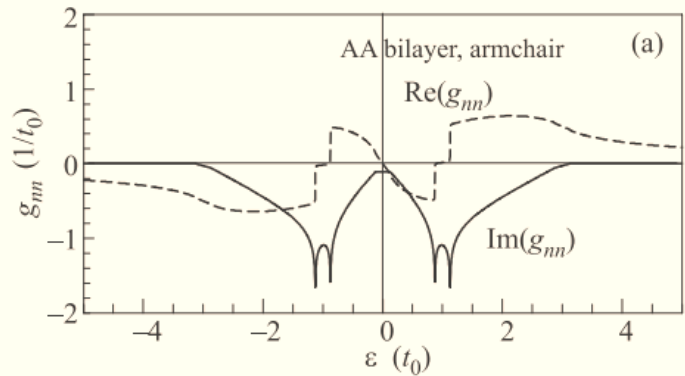
Green's function  
for the contacting atoms



current-voltage curve

current-voltage curve for the  
gate voltage  $V_g = 0.05t_0$ ,  $0.1t_0$ , and  $0.2t_0$

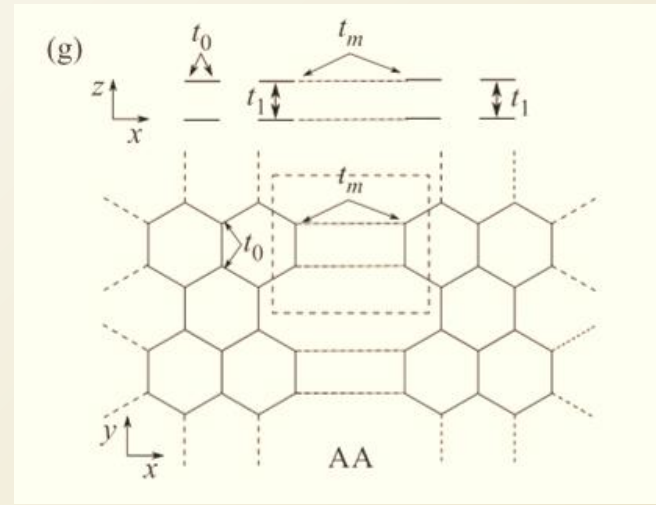
# AA bilayer, armchair



Green's function  
for the contacting atoms

current-voltage curve

current-voltage curve for the  
gate voltage  $V_g = 0.05t_0$ ,  $0.1t_0$ , and  $0.2t_0$

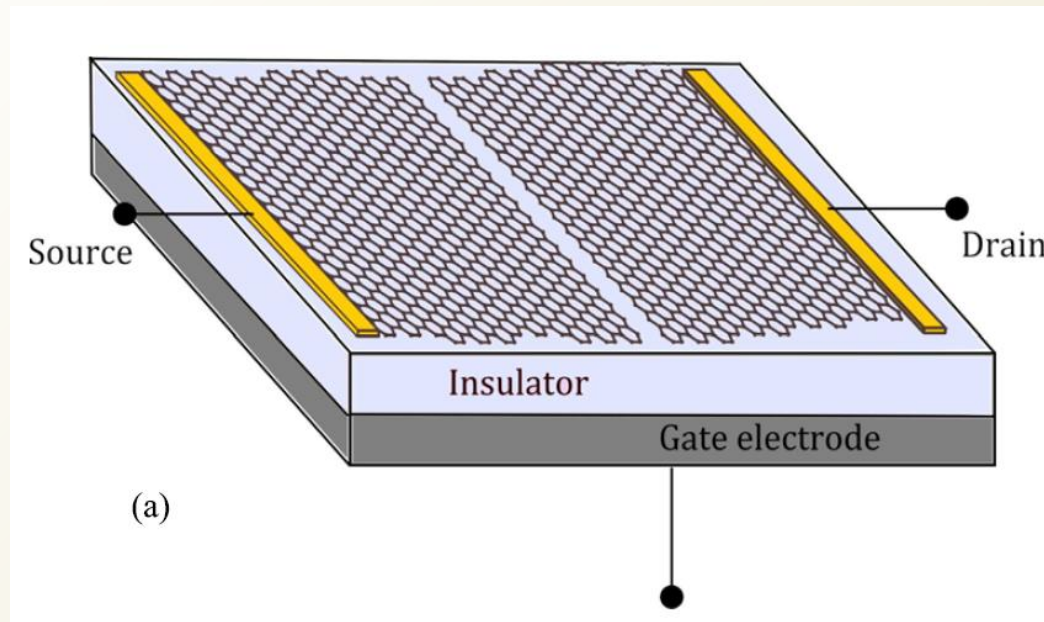


# Conclusion

(1) Using all kinds of graphene based tunnel junctions with zigzag-type edges, **electronic switching devices** can be developed owing to the presence of the localized edge states existing within a narrow energy range.

(2) For the graphene single layer and AB graphene bilayer, these states are located in the vicinity of the Fermi level. At the same time, for the AA graphene bilayer, they are shifted with respect to the Fermi energy by the interlayer coupling parameter. Thus, the first two types of junctions are promising for developing a **device switching off** under the effect of the gate voltage, whereas the junctions of the latter type can be used for **switching on**.

(3) The graphene based junctions with the armchair edges do not exhibit clearly pronounced **switching properties**. Here, the gate voltage can only change the conductivity.



Our novel device demonstrates an original switching mechanism and manifests an interesting region of the negative differential resistivity. There is reason to hope that all these findings may have extensive applications in graphene-based electronics.

**Patent application № RU 2014103818**

**V. L. Katkov and V. A. Osipov, *Planar graphene tunnel field-effect transistor*  
Appl. Phys. Lett. 104, 053102 (2014)**

**В.Л. Катков, В. А. Осипов, *Туннельный контакт на базе графена*  
Письма в ЖЭТФ 98, 782 (2013)**

**Thank you for your attention!**