Electron Transport in Crossed Graphene Nanoribbon Devices: 4-Terminal *ab initio* Simulations

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ABSTRACT

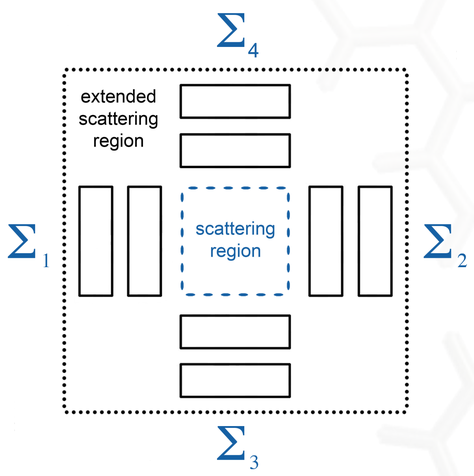
With the aim of exploring the potential of graphene in electronics, a lot of effort has been spent on the energy-gap engineering so to allow having an off state. Recently, it has been reported theoretically a **current switching mechanism by voltage control** in a graphene crossbar made by two 14-armchair nanoribbons (GNRs) rotated by 90° [1].

It has been also recently shown that different stacking in bilayer GNRs leads to significant changes on the electronic properties [2]. Therefore, in order to investigate the possibilities of using crossed GNRs as ON/OFF devices, we have studied the **electronic and transport properties** of those systems **as function of their relative rotation angle and inter-layer distance**.

Our calculations were performed with **TranSIESTA** code [3], which has been recently generalized, based on ref. [4], to consider ***N* ≥ 1 arbitrarily distributed electrodes at finite bias** [5].

METHODOLOGY

NEGF + DFT



$$\begin{pmatrix} \bar{H}_1 & 0 & \bar{H}_{1M} & 0 & 0 \\ 0 & \bar{H}_3 & \bar{H}_{3M} & 0 & 0 \\ \bar{H}_{M1} & \bar{H}_{M3} & \bar{H}_M & \bar{H}_{M4} & \bar{H}_{M2} \\ 0 & 0 & \bar{H}_{4M} & \bar{H}_4 & 0 \\ 0 & 0 & \bar{H}_{2M} & 0 & \bar{H}_2 \end{pmatrix} G^r = \mathbb{1}$$

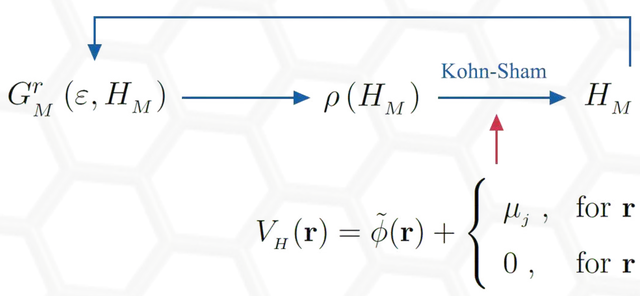
where $\bar{H}_x = \varepsilon S_x - H_x$ with $\varepsilon = \lim_{\eta \to 0^+} E + i\eta$.

$$G^r_M = \left[\varepsilon S_M - H_M - \sum_j \Sigma^r_j \right]^{-1}$$

➡ density dependent Hamiltonian:

$$\rho = \frac{1}{2\pi i} \int_{-\infty}^{+\infty} d\epsilon \, G^<_M = \frac{1}{2\pi} \int_{-\infty}^{+\infty} d\epsilon \, G^r_M \left[\sum_j \Gamma_j f\left(\epsilon - \mu_j\right) \right] G^a_M$$

where $\Gamma_j = i\left[\Sigma^r_j - \Sigma^{r\dagger}_j\right]$, $f\left(\epsilon - \mu_j\right) = f_j$ the Fermi-Dirac distribution.

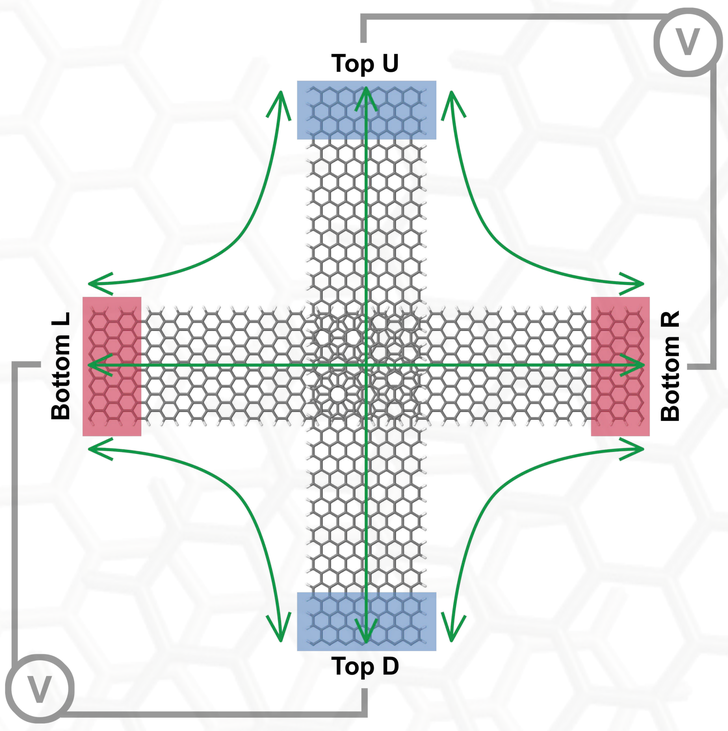


$$V_H(\mathbf{r}) = \tilde{\phi}(\mathbf{r}) + \begin{cases} \mu_j \,, & \text{for } \mathbf{r} \in \mathbf{r}_j \\ 0 \,, & \text{for } \mathbf{r} \notin \mathbf{r}_j \end{cases}$$

➡ current (Büttiker-Landauer):

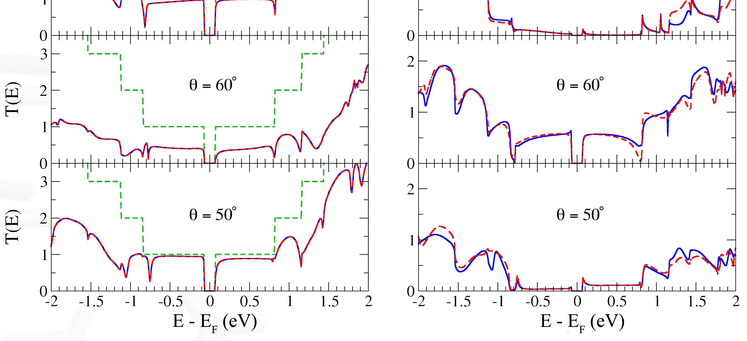
$$I_j = \frac{2e}{h} \sum_{j'} \int_{-\infty}^{+\infty} d\epsilon \, \underbrace{\mathrm{Tr}\left[\Gamma_j G^{r\,\dagger}_M \Gamma_{j'} G^r_M \right]}_{\text{transmission}} \left(f_j - f_{j'} \right)$$

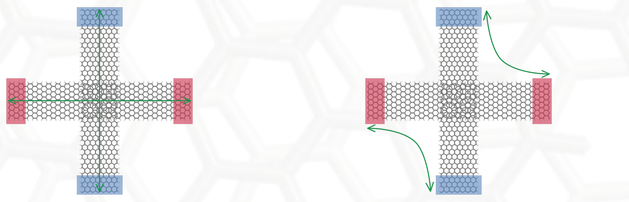
RESULTS

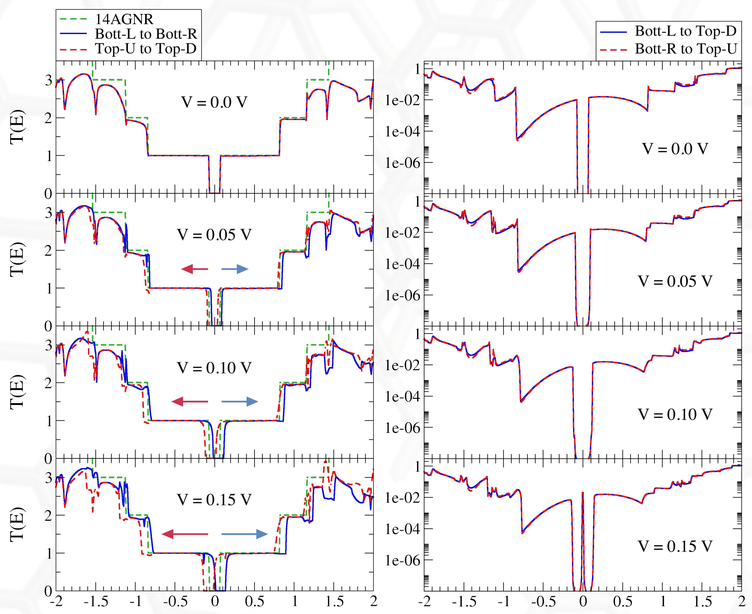


Simulation characteristics:

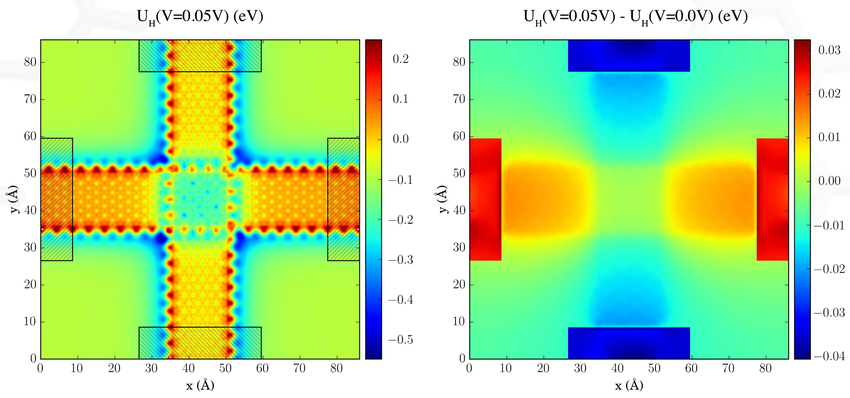
- 1280 atoms;
- double-ζ (9280 orbitals);
- vdW (optB88);
- real space grid cutoff: 350 Ry;
- forces < 5 meV/Å;
- interlayer distance: 3.34 Å (lowest energy).



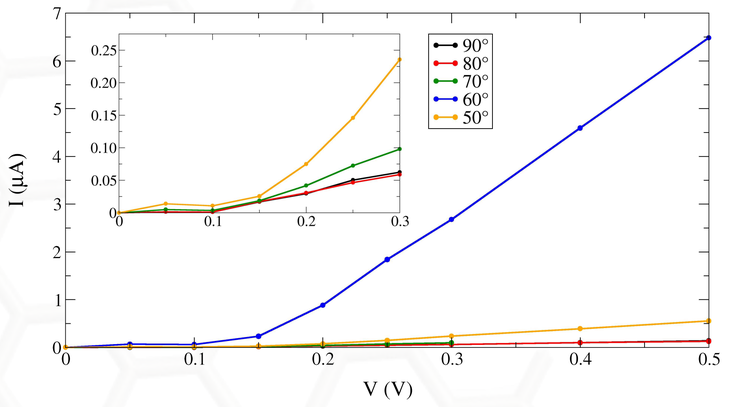




Electrostatic potential at the plane between the ribbons for V = 0.05 V



Bottom-Left to Top-Down



CONCLUSIONS

We find that the transmission along each individual GNR and among them **strongly depends on the stacking**. For a 60° rotation angle, one finds an almost perfect match of the ribbons' honeycomb lattice in the crossing region, resulting in a strong scattering effect that also translates into an increased inter-layer transmission.

REFERENCES

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