

Electronic and Transport Properties of 4-Terminal Crossed Graphene Nanoribbons Devices

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MOTIVATION

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 a **current switching mechanism by voltage control** in a graphene crossbar made by two H-passivated 14-armchair nanoribbons rotated by 90° [1].

Despite of the fast improvement of experimental techniques over the past decade for producing and manipulating graphene nanoribbons, the fabrication of graphene crossbars with a high-precision control on the nanoribbons orientation and relative position is still a difficult task. Moreover, it has been shown that different stacking in graphene bilayer nanoribbons leads to differences on the electronic properties [2].

In this work we study the electronic and the transport properties of crossed graphene nanoribbons systems varying the relative rotation angles and the inter-layer distances. We used the *ab initio* electronic transport code **TranSIESTA** [3], which has been recently generalized to consider **multi-terminal devices** [4].

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 $\varepsilon = \lim_{\eta \rightarrow 0^+} E + i\eta$.

$$G_M^r = \left[\varepsilon S_M - H_M - \sum_j \Sigma_j \right]^{-1}$$

→ density dependent Hamiltonian:

$$\rho = \frac{1}{2\pi} \int dE G_M^r \left[\sum_j \Gamma_j f(E - \mu_j) \right] G_M^r \dagger$$

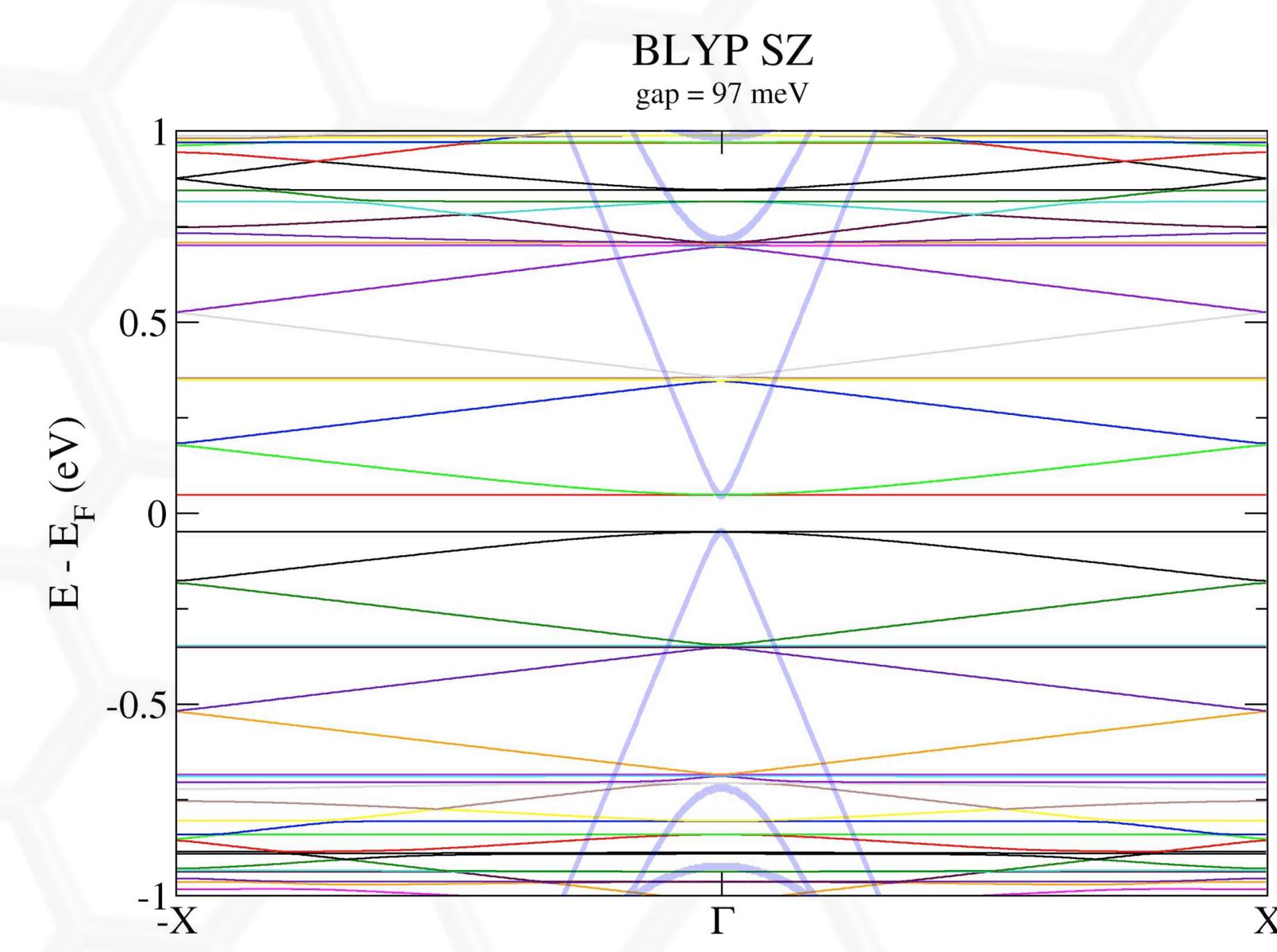
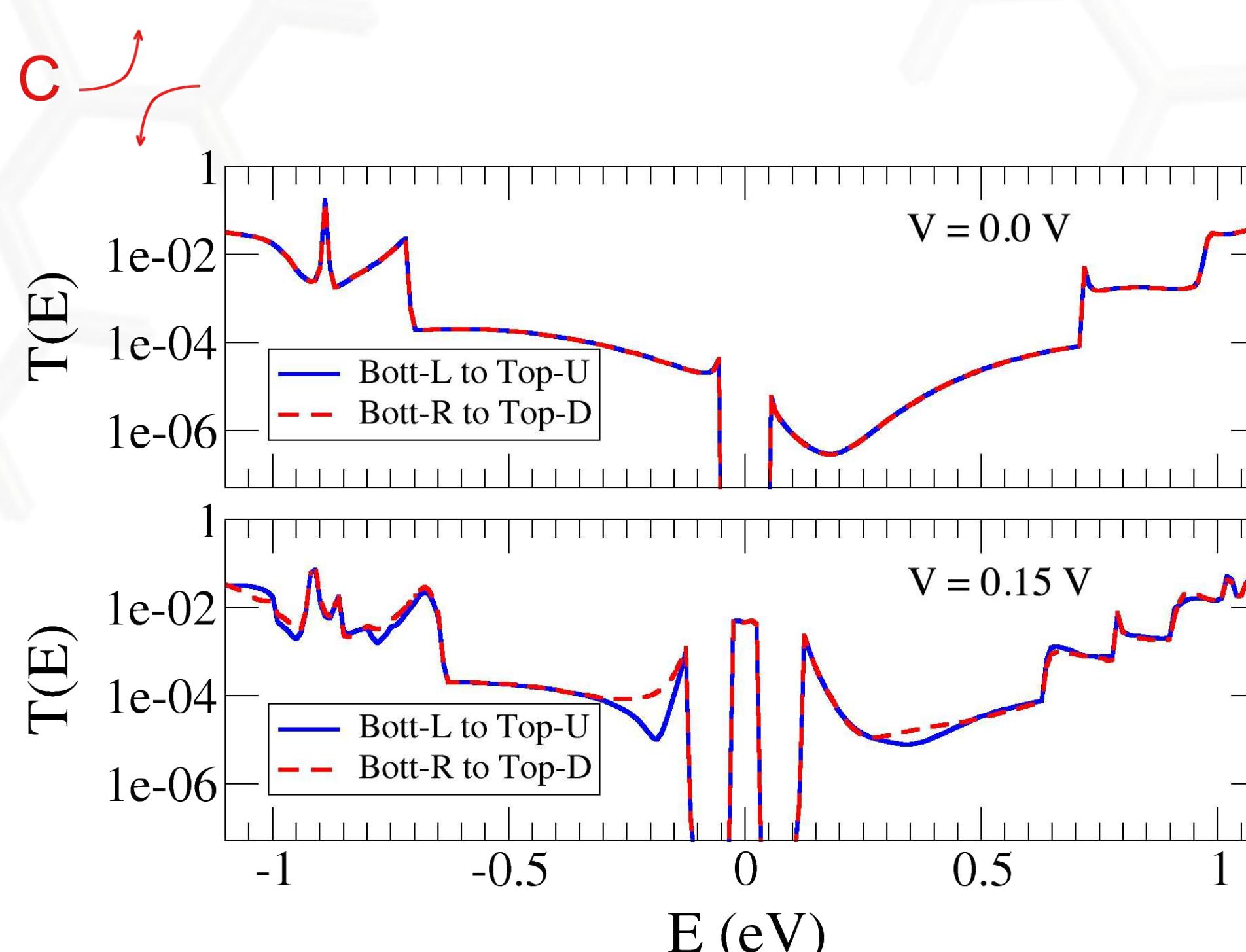
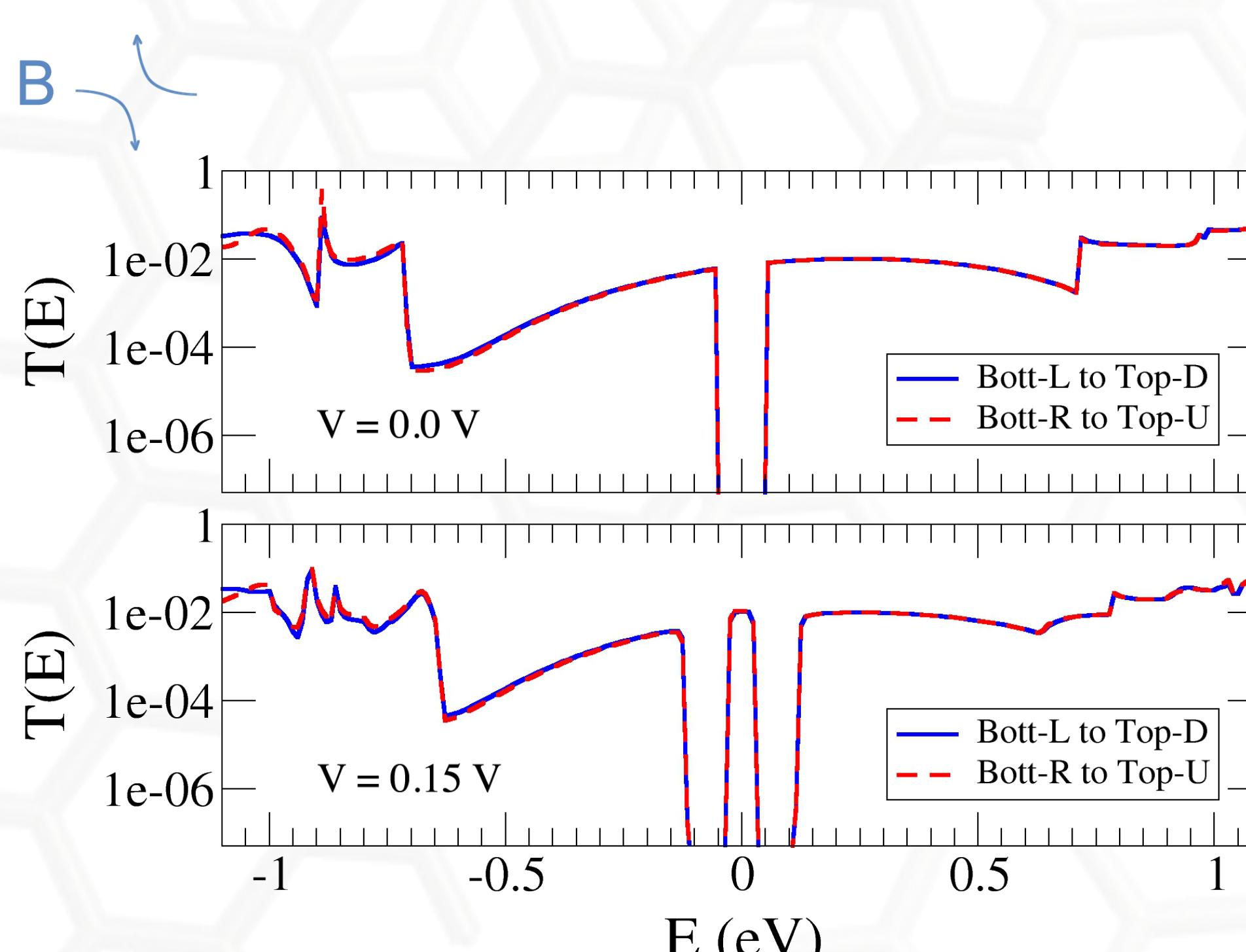
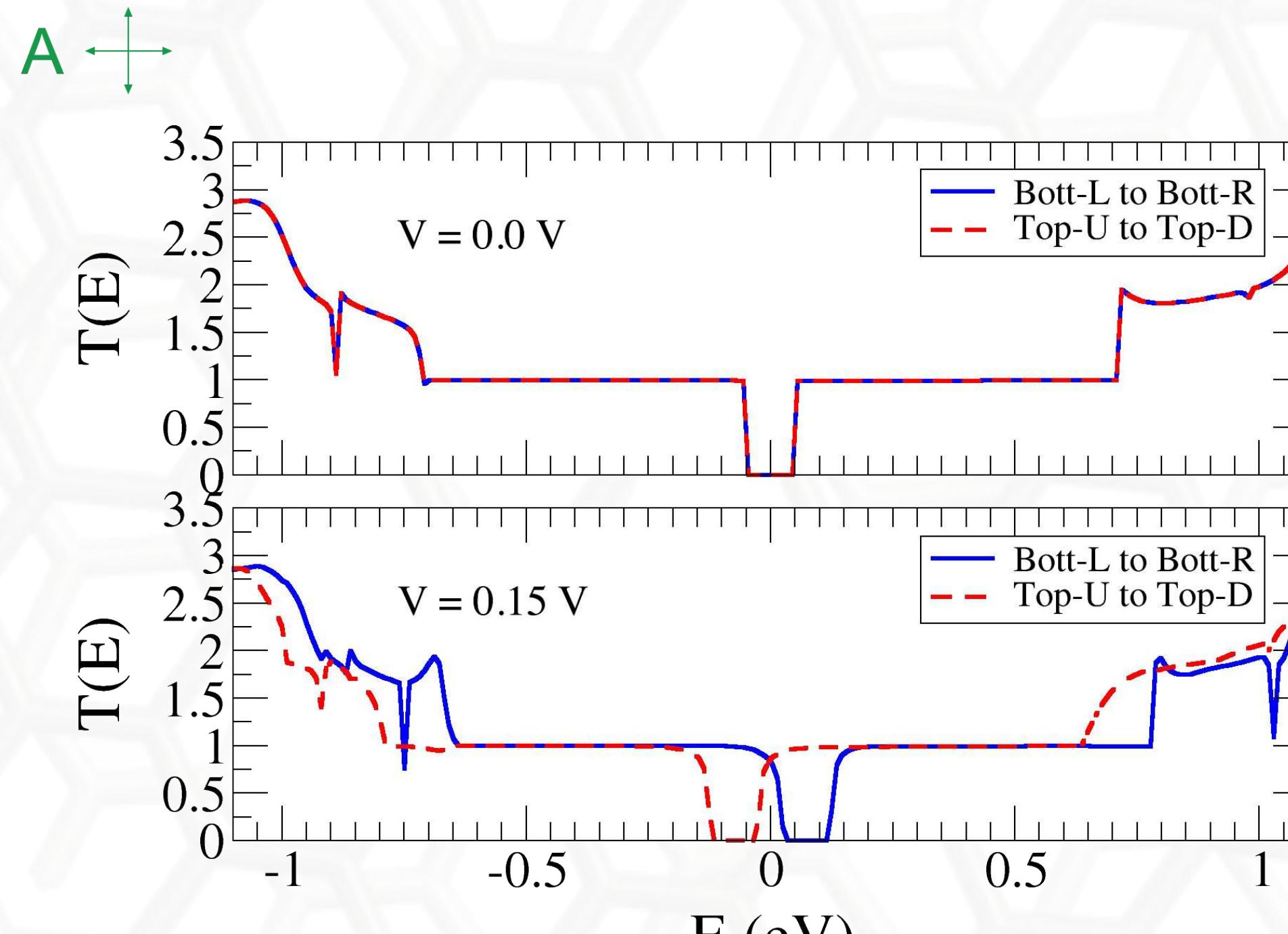
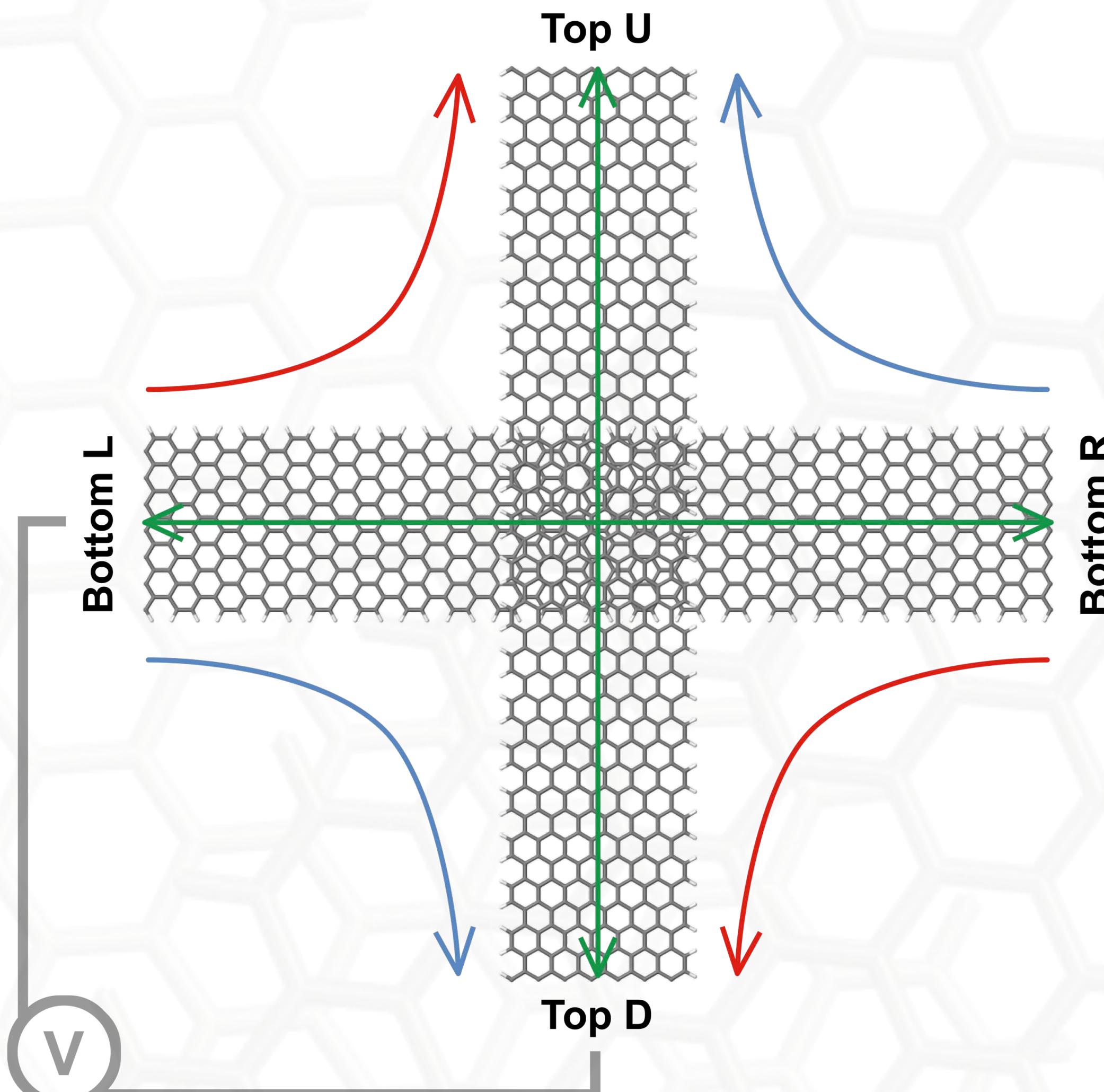
Kohn-Sham

$$G_M^r(\varepsilon, H_M) \longrightarrow \rho(H_M) \longrightarrow H_M(\rho)$$

↓ current

$$I_{ij} = \frac{e}{h} \int dE \text{Tr} [\Gamma_i G_M^r \dagger \Gamma_j G_M^r] (f(E - \mu_i) - f(E - \mu_j))$$

RESULTS



functional	basis set	stacking	lattice constant (Å)		binding energy (eV/atom)
			a	c	
PBE	SZ	AA	2.539	2.985	-0.071
PBE	SZ	AB	2.539	2.781	-0.103
PBE	DZP	AA	2.479	3.865	-0.004
PBE	DZP	AB	2.478	3.698	-0.005
BLYP	SZ	AA	2.549	3.052	-0.042
BLYP	SZ	AB	2.549	2.851	-0.065
BLYP	DZP	AA	2.487	4.089	0.000
BLYP	DZP	AB	2.487	3.970	0.000
LDA	SZ	AA	2.514	2.850	-0.117
LDA	SZ	AB	2.514	2.670	-0.159
LDA	DZP	AA	2.455	3.453	-0.015
LDA	DZP	AB	2.455	3.225	-0.022
VDW	SZ	AA	2.536	2.940	-0.113
VDW	SZ	AB	2.535	2.769	-0.146
VDW	SZP	AA	2.491	3.084	-0.091
VDW	SZP	AB	2.491	2.878	-0.114
VDW	DZ	AA	2.476	3.486	-0.034
VDW	DZ	AB	2.476	3.294	-0.040
VDW	DZP	AA	2.475	3.419	-0.033
VDW	DZP	AB	2.473	3.275	-0.040
graphite		2.462 [5]	3.354 [5]	-0.043 [6]	0.035 (+0.015,-0.010) [7]

CONCLUSIONS

The approach for multi-terminal devices applied to crossed graphene nanoribbons presents satisfactory results, in qualitative agreement with those previously reported in [1].

It was performed a study with different functionals and basis set so to verify which of them would give better results when compared to experimental data.

Next steps will be to verify the changes in the electronic and transport properties when varying the ribbons interlayer distance and their relative angle.

REFERENCES

- [1] K. M. Masum Habib and Roger K. Lake. *Phys. Rev. B* **68**, 045418 (2003).
- [2] H. Santos, A. Ayuela, L. Chico, and Emilio Artacho. *Phys. Rev. B* **85**, 245430 (2012).
- [3] Mads Brandbyge, José-Luis Mozo, Pablo Ordejón, Jeremy Taylor, and Kurt Stokbro. *Phys. Rev. B* **65**, 165401 (2002).
- [4] Kamal K. Saha and Wenchang Lu and J. Bernholc and Vincent Meunier. *J. Chem. Phys.* **131**, 164105 (2009).
- [5] You Xiang Zhao and Ian L. Spain. *Phys. Rev. B* **40**(2), 993 (1989).
- [6] L. A. Girifalco and R. A. Lad. *J. Chem. Phys.* **25**, 693 (1956).
- [7] Lorin X. Benedict, Nasreen G. Chopra, Marvin L. Cohen, A. Zettl, Steven G. Louie, and Vincent H. Crespi. *Chem. Phys. Lett.* **286**, 490 (1998).

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