

Toward all-carbon nanodevices: experimental synthesis, transport characterization and modelling

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Abstract

Graphene nanoribbons (GNRs) are promising candidates for novel electronic devices: they overcome the low on/off-behaviour of graphene while still preserving high charge carrier mobility that is essential for the fabrication of efficient field effect transistors. Atomically precise GNRs can be fabricated by an on-surface synthesis approach [1]. In this work, we characterize the electronic transport properties of an all-carbon GNR-based device (sketched in Fig. 1) realized experimentally in our laboratory together with similar devices [2]. We simulate a selection of configurations to understand the relationship between the behaviour of the device and its underlying atomic structure.

This presentation will focus on quantum transport calculations carried out with the OMEN Software [3] in the framework of the Non-Equilibrium Green's Function formalism (NEGF) and takes advantage of ab-initio DFT Hamiltonians produced by the CP2K code [4]. Particular attention will be set on quantifying the impact of the spatial orientation of the channel GNRs on the ON-set current (see Fig. 2). Moreover, we will analyse how the presence of geometrical defects at the contact edge and/or in the bridging GNRs, as well as the morphology of the lead edges, influence the device

performance. Finally, dissipative phase-breaking processes induced by electron-phonon interaction will be considered in the transport characterization.

References

- [1] J. Cai et al., *Nature* 466, (2010), 470
- [2] L. Martini et al., *Carbon* 146, (2019) 36.
- [3] M. Luisier et al., 8th IEEE Conference on Nanotechnology IEEE, (2008).
- [4] CP2K: <https://www.cp2k.org>.

Figures

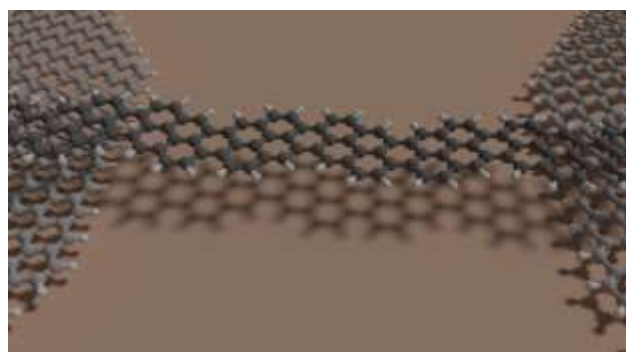


Figure 1: Schematic representation of the all-carbon GNR-based device realized experimentally.

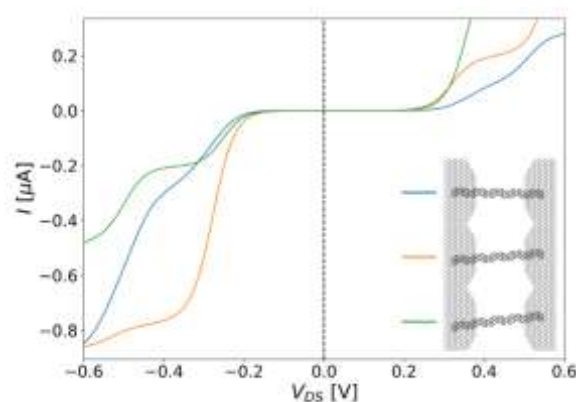


Figure 2: Current-voltage characteristics for different orientations of the channel GNRs.