# Currents in Fluroinated Graphene

### Electron Transport in 1D Fluorine Saturated Graphene Materials

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## In Short

- Using the electronic properties of fluorine saturated graphene material to construct interesting transport models.
- Exploring the impact of the width of the ZGNRs and the fluorination degrees on the transport properties.

Depending on the fluorinating reaction time on graphene materials, the stoichiometry of carbon and fluorine atoms could be tuned. These resulted materials have a wide range of electronic properties. [1] Experimentally successful synthesis of fluorinated graphene materials via electron beam has been carried out. The measurements on the materials reveal their global conductivities depend strongly on the size of the fluorination area in the system [2]. In this project, we intend to understand transport properties and detailed electron migration path of fluorinated graphene materials. In this spirit, 1D fluorine saturated nanoribbons (GNRs) based transport models will be constructed. (see Fig.1) Two factors in the scattering region of interest will be taken into account: 1 the width of the GNRs and 2. the fluorination degrees, which simulate the variation of the fluorination area. Based on the electronic properties of 1D GNRs materials, the global transport properties at quasi-stationary limit for different transport models will be investigated.

Our primarily results on 6ZGNRs transport models

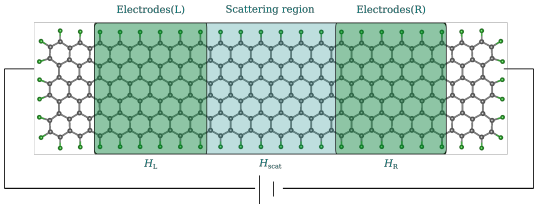


***Figure 1:** Representation of a transport model based on edge fluorinated Zigzag-GNRs. Carbon atoms are drawn in black, the fluorine atoms are in green. The nanojunction is partitioned into three parts: the central scattering region and two electrodes parts (L/R). The outer fluorine atoms and first two slices of edge carbon atoms are neglected in the construction of the complete system Hamiltonian, which are not included in the color boxes. The electrodes part of the transport Hamiltonians shown in the green boxes are repeated to mimic the required semi-infinite electrodes.*

reveal the potential spintronics application, where $\alpha$ and $\beta$ channels behave differently. Combining our implementation on local current density [3] within Non-Equilibrium Green's Function framework, detailed transport mechanism can be revealed (see Fig.2) In our best hope, the results will help us draw insight on the detailed structure-function relation, which potentially assists the design of new transistors based on fluorinated graphene materials.

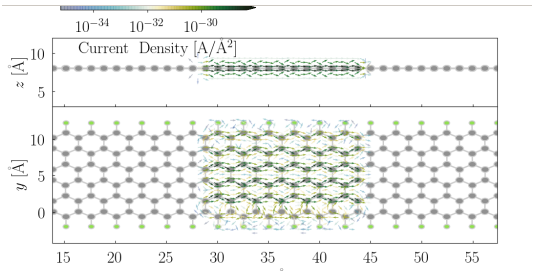


***Figure 2:** Quiver plot of the electronic current density projected on a real space grid. The local currents on the scattering region are reported for pristine 6ZGNRs. A 1V bias voltage along the $x$-axis of the nanojunction plane is applied. For simplification, the current density is integrated along the $y$-axis of the nanojunction plane for the side view and the top view is integrated along the $z$-axis. The intensity of the current density is illustrated according to the color bar, where green indicates the high intensity and blue presents the low intensity.*

## WWW

http://www.bcp.fu-berlin.de/chemie/

## More Information

[1] J. T. Robinson, J. S. Burgess, C. E. Junkermeier, S. C. Badescu, T. L. Reinecke, F. K. Perkins, M. K. Zalalutdniov, J. W. Baldwin, J. C. Culbertson, P. E. Sheehan, et al., *Nano. letters.* **10**, 3001 - 3005 (2010).

[2] F. Withers, T. H. Bointon, M. Dubois, S. Russo, M. F. Craciun, *Nano. letters.* **11**, 3912 - 3916 (2011).

[3] J. Shao, V. Pohl, L. E. Marsoner Steinkasserer, B. Paulus, J. C. Tremblay, *J. Phys. Chem. C* (2020).