(One page abstract format: including figures and references. Please follow the model below.)

Correlating electrical measurements of carbon nanostructures inside the TEM with first principles calculations

Andrés R. Botello-Méndez[1], O. Cretu[2], A. La Torre[2], Z. J. Qi[3], J. A. Rodríguez-Manzo[3], M. Drndić[3], A. T. C. Johnson[3], F. Banhart[2], J.-C. Charlier[1]

[1]IMCN-NAPS Université catholique de Louvain, Chemin des étoiles 8, 1348 Louvain la neuve, Belgium
andres.botello@uclouvain.be
[2]Institut de Physique et Chimie des Matériaux de Strasbourg, UMR 7504 CNRS, University of Strasbourg, 23 rue du Loess, 67034 Strasbourg
[3]Department of Physics and Astronomy, University of Pennsylvania, Philadelphia, Pennsylvania 19104, USA.

Abstract

The interest of carbon nanostructues as potential active or passive components in next generation electronics is in great part due to the large range of properties that these systems exhibit. For instance, it has been shown theoretically that the electronic structure of carbon nanotubes (CNTs) and carbon nanoribbons (CNRs) strongly depend on the details of their atomic structure. This represents both an opportunity to tailor the electrical properties and a challenge to achieve atomically precise synthesis and characterization. In particular, the electrical characterization of carbon nanostructures has been elusive due to the challenging task of having accurate information of both the atomic structure and the electrical response.

Recent breakthroughs in the spatial resolution of electron microscopes and the possibility to make electrical measurements inside them have provided unprecedented information about the electrical behaviour of these systems. Coupled with simulations, important contributions to the understanding of the electrical behaviour of carbon nanostructures have been made.

Here, the specific examples of the electronic characterization of atomic chains of carbon and CNRs are used to compare with transport calculations based on first-principles DFT and tight biniding models [1-3]. The qualitative agreement between experiment and simulation allow a solid understanding of the properties of these systems. However, the quantitative discrepancies offer challenges on both sides.

References

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[2] Z.J. Qi, J.A. Rodríguez-Manzo, A.R. Botello-Méndez, S.J. Hong, E.A. Stach, Y.W. Park, J.-C. Charlier, M. Drndić, A.T.C. Johnson, Nano Lett. **14** (2014) 4238.
[3] A. La Torre, A.R. Botello-Mendez, J.-C. Charlier, F. Banhart, Nature Comm. (2014) *submitted*.

Figures

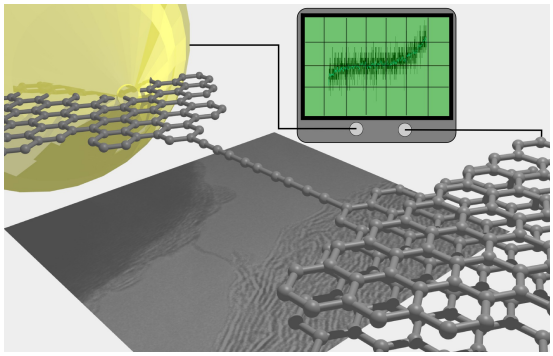

Figure 1: Schematic view of the transport through a carbon chain inside the TEM