

Transport Properties in Disordered Graphene: Effects of Atomic Hydrogen and Structural Defects

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This talk will focus on the presentation of transport properties in graphene-based-materials, driven by chemical functionalization and structural defects. To circumvent the current hurdles preventing the advent of graphene nanoelectronics, it has become urgent to benefit from engineering complexity at the nanoscale and the unique potential of graphene as a bridging platform between top-down conventional CMOS technologies and (bio)-chemistry self-assembling processes.

Here, by using state-of-the-art multiscale simulations (combining first-principles with tight-binding schemes), we present several electronic transport features in complex forms of chemically modified graphene based materials. Past examples include the use of boron or nitrogen-doped to produce graphene-based nanoribbons exhibiting “mobility gaps” of width as large as 1eV, providing an efficient switching behavior principle even in the presence of a vanishing electronic band-gap. The possibility to design a switching effect based on mechanical deformation of graphene nanoribbons. Here, we will explore the effect of atomic hydrogen driving intrinsic magnetic ordering will be presented from a theoretical perspective and in comparison with most recent experiments.

It will be shown that the existence of a long range ferromagnetic state in weakly hydrogenated graphene could be related to a highly robust metallic state down to cryogenic temperatures, in contrast to the localization regime obtained in absence of ferromagnetic order. Additionally, the possibility to observe measurable magnetoresistance signals due to magnetism in graphene will be discussed. As a second issue, the presence of structural defects will be shown to yield conventional localization effects.

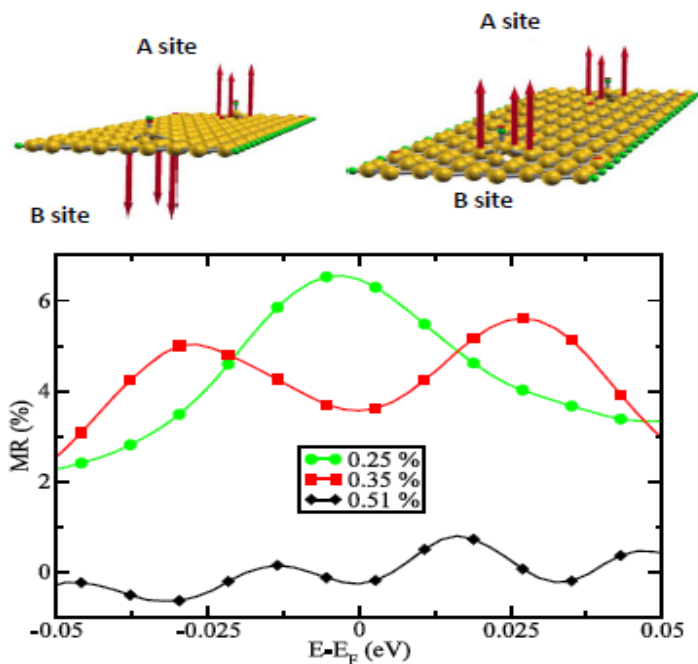


Figure: Magnetoresistance of a weakly hydrogenated graphene sample predicted numerically.

Related bibliography

Mark H. Rummeli et al., *Graphene: Piecing it Together*, **Advanced Materials**, 23, 4471–4490 (2011)

F. Ortmann, A. Cresti, G. Montambaux and **S. Roche**, *Magnetoresistance in disordered graphene: The role of pseudospin and dimensionality effects unravelled*, **European Physics Letters**, 94, 47006 (2011)

D. Soriano, N. Leconte, P. Ordejon, J.-Ch. Charlier, J.-J. Palacios, and **S. Roche**, *Magnetoresistance and Magnetic Ordering Fingerprints in Hydrogenated Graphene*, **Physical Review Letters** 107, 016602 (2011)

A. Lherbier, S.M.M. Dubois, X. Declerck, Sr. Roche, Y.-M. Niquet and J.C. Charlier, *Two-dimensional Graphene with Structural Defects: Elastic Mean Free Path, Minimum Conductivity and Anderson* **Physical Review Letters**, 106, 046803 (2011)

N. Leconte, D. Soriano, **S. Roche**, P. Ordejon, J.-Ch. Charlier, and J. J. Palacios *Magnetism-Dependent Transport Phenomena in Hydrogenated Graphene: From Spin-Splitting to Localization Effects* **ACS Nano** 5, 3987 (2011); DOI: 10.1021/nn200558d

A. Cresti, A. Lopez-Bezanilla, P. Ordejon and **S. Roche** *Oxygen surface functionalisation of graphene nanoribbons for transport gap engineering* **ACS Nano**, DOI: 10.1021/nn203573y (2011)