Chemical edge engineering of Graphene Nano Ribbons: a DFT study

Ph. Wagner[1]**,** A. Pateau[1], A. López-Bezanilla[2], S. Roche[3,4]**,** P. R. Briddon[5], C. P. Ewels[1]

[1] Institute of Materials, CNRS, Université de Nantes, BP32229, 44322 Nantes, France
[2] Oak Ridge National Laboratory, PO Box 2008, Oak Ridge, TN 37831, U.S.A.
[3] CIN2 (ICN-CSIC) and Universitat Autonoma de Barcelona, Catalan Institute
of Nanotechnology, Campus de la UAB, 08193 Bellaterra (Barcelona), Spain
[4] ICREA, Institució Catalana de Recerca i Estudis Avançats, 08010 Barcelona, Spain
[5] Department of Electrical Engineering, Newcastle University, Newcastle Upon Tyne, U.K.
philipp.wagner@cnrs-imn.fr

Although graphene displays a large number of extraordinary properties, there is still a need to modify some of these for graphene based devices. Notably for transistor design it is necessary to create and engineer an electronic gap in graphene. One way to introduce such a gap is by cutting graphene into graphene nanoribbons (GNRs). Previous studies have shown that ribbon gaps decrease exponentially with increasing width [1]. However less attention has been paid to other ways of controlling the band gap of ribbons. In particular, structure and chemical design of edge states are beginning to receive attention [2]. First experiments have shown that the most stable configurations of GNRs with chemically functionalised edges are mostly either zigzag or armchair edges [3]. The simplest chemical edge termination of GNRs is hydrogen termination, which is used almost exclusively in theoretical modeling [4,5]. In experiments however edges will be commonly terminated by a range of species including N, O, etc. Depending on the functional group both the electronic structure and the surface topology can change, as recently proposed in calculations of twisted F-terminated GNRs [6].

We present here the result of theoretical DFT studies of OH-terminated armchair and zigzag GNRs, and show first evidence of the stability of 3D-rippled edges as compared to flat OH-terminated ribbons. GNR result in a significant change of the GNR band gap as compared to equivalent hydrogen terminated ribbons. Hydrogen bonding occurs between neighbouring edge functional groups. We discuss resultant mobility and transport properties and the possibility for band gap and transport engineering through chemical control of edge site terminations.

References

[1] V. Barone, O. Hod, G. E. Scuseria, Nano Lett. **6** (12), (2006) 2748
[2] C. K. Gan and D. J. Srolovitz, Phys. Rev. B, **81**, (2010) 125445
[3] T. Wassmann, A. Seitsonen, A. Saitta, M. Lazzeri, F. Mauri, Phys. Rev. Lett., **101**, (2008) 096402
[4] Y. Kobayashi, K. Fukui, T. Enoki, K. Kusakabe, and Y. Kaburagi, Phys. Rev. B, **71**, (2005) 193406
[5] K. Nakada, M. Fujita, G. Dresselhaus, and M. S. Dresselhaus, Phys. Rev. B, **54**, (1996) 17954
[6] D. Gunlycke, J. Li, J. W. Mintmire, and C. T. White, Nano Lett., **10**, (2010) 3638