Damaging Graphene with Ozone Treatment : a Chemically Tunable Metal-Insulator Transition

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We present an *ab initio* multiscale study of electronic and transport properties of two- dimensional graphene after epoxide functionalization via ozone treatment[1,2]. The orbital rehybridization induced by the epoxide groups triggers a strong intervalley scattering and changes dramatically the conduction properties of graphene. A DFT-parametrized tight-binding model within the Kubo formalism[3] allows us to simulate mesoscopic-sized systems up to 2 million atoms. By varying the random coverage density of epoxide defects from 0.1 to 4%, charge conduction can be tuned from a diffusive to a strongly localized regime, with localization lengths down to a few nanometers long. Experimental results[4] supporting the interpretation as a metal-insulator transition are also provided.

References

[1] N. Leconte, J. Moser, P. Ordejon, H. Tao, A. Lherbier, A. Bachtold, F. Alsina, C.M. Sotomayor Torres, J.-C. Charlier, and S. Roche, submitted to ACS Nano (2010)
[2] N. Leconte, P. Ordejon, A. Lherbier, J.-C. Charlier, and S. Roche (in preparation)
[3] H. Ishii, F. Triozon, N. Kobayashi, K. Hirose, and S. Roche, C. R. Physique **10**, 283 (2009)
[4] J. Moser, H. Tao, S. Roche, F. Alsina, C.M. Sotomayor Torres, and A. Bachtold, arXiv:1003.1299

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