Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Ab initio quantum transport in N-doped graphene JEAN-CHRISTOPHE CHARLIER, ANDRÉS R. BOTELLO-MÉNDEZ, AURÉLIEN LHERBIER, University of Louvain, Institute of Condensed Matter and Nanosciences (Belgium), NAPS TEAM — Electronic structure and transport properties of N-doped graphene with a single sublattice preference [1] are then investigated using both first-principles techniques and a real-space Kubo-Greenwood approach [2]. Such a breaking of the sublattice symmetry leads to the appearance of a true band gap in graphene electronic spectrum even for a random distribution of the N dopants. In addition, a natural spatial separation of both types of charge carriers at the band edge is observed, leading to a highly asymmetric electronic transport. For such N-doped graphene systems, the carrier at the conduction band edge present outstanding transport properties including long mean free paths, high mobilities and conductivities. Such a transport behavior can be explained by a non-diffusive regime (quasi-ballistic transport behavior at the conduction band edge), and originates from a low scattering rate [2]. The presence of a true band gap along with the persistence of carriers traveling in an unperturbed sublattice suggest the use of such N-doped graphene in G-FET applications, where a high Ion/Ioff ratio is expected.

[1] R. Lv, Q. Li, A.R. Botello-Mendez, et al. Nature - Scientific Reports 2, 586 (2012).
[2] Electronic and transport properties of unbalanced sublattice N-doping in graphene, A. Lherbier, A.R. Botello-Méndez, and J.-C. Charlier, Nano Lett. 13, 1446-1450 (2013).

Jean-Christophe Charlier
University of Louvain, Institute of Condensed Matter
and Nanosciences (Belgium)

Date submitted: 11 Nov 2014 Electronic form version 1.4