Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

1-D Quantum Well States on Doped Graphene Nanoribbons Revealed by Transport Simulations[1] P. BRANDIMARTE, CFM CSIC-UPV/EHU, Spain, E. CARBONELL-SANROMÀ, CIC nanoGUNE, Spain, R. BALOG, Aarhus University, Denmark, M. CORSO, CIC nanoGUNE, Spain, S. KAWAI, Uni Basel, Switzerland, A. GARCIA-LEKUE, DIPC, Spain, S. SAITO, Kyoto University, Japan, S. YAMAGUCHI, ItbM, Japan, E. MEYER, Uni Basel, Switzerland, J. I. PASCUAL, CIC nanoGUNE, D. SÁNCHEZ-PORTAL, CFM CSIC-UPV/EHU, Spain — Quantum-well states have recently been observed in scanning tunneling microscopy experiments with chemically functionalized armchair graphene nanoribbons (AGNRs), more specifically on pristine segments confined by pairs of boron-substituted atoms into the AGNR backbone.[2] Here we present a first-principles study of the electronic and transport properties of such doped AGNRs. Our results reveal that the boron pairs selectively confine the first valence band of the pristine AGNR while being almost transparent for the second one. Such band-dependent electron scattering is explained in terms of the symmetry matching between the electronic wave functions of states from the pristine AGNRs and those localized at the boron pairs. Our simulations not only reproduce the experimental measurements but also reveal the mechanism behind the observations.

[1]FP7FET-ICT PAMS-project (European Commission, contract 610446), MINECO (grant MAT2013-46593-C6-2-P) and Basque Dep. de Educación, UPV/EHU (grant IT-756-13).
[2]E. Carbonell-Sanromà *et al*, submitted.

Pedro Brandimarte
CFM CSIC-UPV/EHU

Date submitted: 11 Nov 2016 Electronic form version 1.4