Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Theory of Magnetic Edge States in Chiral Graphene Nanoribbons

RODRIGO CAPAZ, Instituto de Fisica, Universidade Federal do Rio de Janeiro, OLEG YAZYEV, STEVEN LOUIE, Department of Physics, U. C. Berkeley and Materials Sciences Division, Lawrence Berkeley National Laboratory — Using a model Hamiltonian approach including electron Coulomb interactions, we systematically investigate the electronic structure and magnetic properties of chiral graphene nanoribbons. We show that the presence of magnetic edge states is an intrinsic feature of any smooth graphene nanoribbons with chiral edges, and discover a number of structure-property relations. Specifically, we describe how the edge-state energy gap, zone-boundary edge-state energy splitting, and magnetic moment per edge length depend on the nanoribbon width and chiral angle. The role of environmental screening effects is also studied. Our results address a recent experimental observation of signatures of magnetic ordering at smooth edges of chiral graphene nanoribbons and provide an avenue towards tuning their properties via the structural and environmental degrees of freedom. This work was supported by National Science Foundation Grant No. DMR10-1006184, the U.S. Department of Energy under Contract No. DE-AC02-05CH11231 and the ONR MURI program. RBC acknowledges financial support from Brazilian agencies CNPq, FAPERJ and INCT-Nanomateriais de Carbono.

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Date submitted: 19 Nov 2010 Electronic form version 1.4