Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Electron Transport Variability in Armchair Graphene Nanoribbons SHELA ABOUD, Stanford University, MASSIMO FISCHETTI, University Texas Dallas — Armchair graphene nanoribbons (AGNR) hold great promise in nano-electronics because of the capability of opening a semiconducting gap in narrow ribbons. However the effective use of AGNR in devices may be limited by structural and chemical modifications from a variety of sources including the support material, edge effects, width variability, and defects which all change the trends in the bandgap scaling. In this work we use density functional theory (DFT) simulations and Empirical Pseudopotentials (EPs) to investigate how structural and chemical variability in the AGNRs influence electron transport through changes in the bandstructure, phonon modes and electron-phonon coupling. Comparisons of the DFT and EPs give the same trend for ribbons with widths of 3N, 3N+1 and 3N+2 atoms with small differences stemming from the atomic structural relaxation accounted for in the DFT simulations. The dependence of the gap on the ribbon width is attributed to the aromaticity of the graphene that can be understood through the spatial distribution of the Clar resonance structures (Clar sextets) and become more localized because of the formation of the edge states. Chemical functionalization of the edges, defects at the edges and in the bulk of the ribbon, doping, and the type of support material (e.g. h-BN, SiO2, HfO and Al2O3) will all modify the aromaticity of the ribbons.

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Date submitted: 28 Nov 2012 Electronic form version 1.4