

Abstract Submitted  
for the MAR15 Meeting of  
The American Physical Society

**Electron and Optical Spectroscopies of Graphene Nanoribbons on Au(111): Insights from Ab-Initio Calculations** ANDREA FERRETTI, SHUDONG WANG, DEBORAH PREZZI, S3 Center, Istituto Nanoscienze, I-41125, Modena, Italy, ALICE RUINI, ELISA MOLINARI, University of Modena and Reggio Emilia, FIM dept & S3 Center, Istituto Nanoscienze, I-41125, Modena, Italy — Narrow graphene nanoribbons (GNRs) exhibit substantial electronic band gaps and optical properties expected to be fundamentally different from the ones of their parent material graphene. Unlike graphene the optical response of GNRs may be tuned by the ribbon width and the directly related electronic band gap. In this work we perform ab initio calculations and compute quasiparticle energies and optical properties of GNRs within the so-called GW-BSE scheme. We focus on a specific armchair nanoribbon (7-AGNR). The presence of the substrate is accounted for by means of a classical image charge model for the screened Coulomb interaction. Our findings show that the metallic substrate induces a significant reduction of the energy gap as compared to the isolated 7-AGNR, bringing the GW gap from  $3.7 \pm 0.1$  eV to 2.3-2.7 eV on Au(111). On the contrary, the position of the optical peaks remains unaltered. Our results are in very good agreement with the experimental values obtained by STS, ARPES, and differential reflectance data, indicating that this scheme can provide quantitative predictions for electron and optical spectroscopies of nanoribbons on weakly coupled substrates such as Au.

Andrea Ferretti  
S3 Center, Istituto Nanoscienze, I-41125, Modena, Italy

Date submitted: 14 Nov 2014

Electronic form version 1.4