Abstract Submitted for the MAR17 Meeting of The American Physical Society

Electronic and Optical properties of Graphene Nanoribbons¹ ELISA MOLINARI, Department of Physics, Mathematics, and Informatics, University of Modena and Reggio Emilia CNR-NANO, 41125 Modena, Italy, AN-DREA FERRETTI, CLAUDIA CARDOSO, DEBORAH PREZZI, S3 Center, Istituto Nanoscienze, I-41125, Modena, Italy, ALICE RUINI, Department of Physics, Mathematics, and Informatics, University of Modena and Reggio Emilia CNR-NANO, 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. We have addressed the optical properties of chevron-like and finite-size armchair nanoribbons by computing the fundamental and optical gap from ab initio methods. Our results are in very good agreement with the experimental values obtained by STS, ARPES, and differential reflectance spectroscopy, indicating that this computational scheme can be quantitatively predictive for electronic and optical spectroscopies of nanostructures.

 $^1{\rm These}$ study has been partly supported by the EU Centre of Excellence "MaX - MAterials design at the eXascale"

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

Date submitted: 07 Feb 2017

Electronic form version 1.4