Abstract Submitted
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Optical properties of graphene nanostructures from first-principles: from 1D to 0D DANIELE VARSANO, DEBORAH PREZZI, S3-CNR, Modena, Italy, ALICE RUINI, ELISA MOLINARI, University of Modena & S3-CNR, Italy — The possibility of patterning graphene sheets in a controllable manner to design semiconducting low-dimensional nanostructures opens exciting opportunities also in view of novel phenomena occurring under light excitation as well as nanoscale optoelectronics applications. We discuss the main characteristics of optical excitations in quasi-1D armchair graphene nanoribbons (A-GNRs) by means of ab-initio many-body calculations [1]. Our theoretical approach includes both self-energy corrections and excitonic effects through the GW-BSE formalism, providing full understanding of excited-state properties. Electron-hole interaction is found to suppress the van Hove singularities -as known for other 1D systems- and introduces strongly bound excitonic peaks. Starting from these ideal structures, we discuss the effect of width modulation on confinement and optical response [2]. Our results show that edge-modulated A-GNRs are efficient systems for the creation of carbon-based QD structures with prominent exciton localization features. [1] D. Prezzi, D. Varsano, A. Ruini, A. Marini, and E. Molinari, Phys. Rev. B 77, 041404 (2008). [2] D. Prezzi, D. Varsano, A. Ruini, and E. Molinari, to be published (2009)

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