Abstract Submitted for the MAR16 Meeting of The American Physical Society

Optical properties of graphene nanoribbons¹ FARHAD KARIMI, IRENA KNEZEVIC, Univ of Wisconsin, Madison — We calculate the dielectric function and optical conductivity of ultra-narrow armchair graphene nanoribbons (AGNRs) and zigzag graphene nanoribbons (ZGNRs) by a self- consistent-field approach within a Markovian master-equation formalism (SCF-MMEF) coupled with full-wave electromagnetic equations. Based on third-nearest-neighbor tight-binding, with appropriate modifications for AGNRs and ZGNRs, we calculate electron dispersions and Bloch wave functions in excellent agreement with the local spin-density approximation (LSDA) results. A generalized Markovian master equation of the Lindblad form, which maintains the positivity of the density matrix, is derived to describe the interaction of the electronic system with an external electromagnetic field (to first order) and with a dissipative environment (to second order). Not only does the SCF-MMEF capture the interband electron-hole-pair generation, but it also accurately accounts for concurrent interband and intraband electron scattering with phonons and impurities. We employ the SCF-MMEF to calculate the dielectric function, complex conductivity, and loss function for both suspended and supported AGNRs and ZGNRs with different widths. Then, we obtain the plasmon dispersion and propagation length from the loss-function maximum.

¹Support by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under Award DE-SC0008712

Farhad Karimi Univ of Wisconsin, Madison

Date submitted: 06 Nov 2015

Electronic form version 1.4