Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Electronic and thermal transport in carbon nanostructures: the role of low-frequency modes NICOLA BONINI, NICOLA MARZARI, Department of Materials Science and Engineering, Massachusetts Institute of Technology — Low-frequency phonon modes play an important role in the electronic and thermal transport properties of carbon nanotubes and ultrathin graphitic films. Not only they determine the very high thermal conductivity of these materials, but they also affect the electrical transport: at low bias they weakly scatter electrons, while at high bias they concur to determine the population of those optical phonon modes that most strongly limit the electrical conductivity. Quite interestingly, these low frequency phonons are also expected to couple to the vibrational modes of a surrounding medium more efficiently than high frequency phonons, providing an effective channel for the exchange of vibrational energy between the nanostructure and the environment. Here we use density functional theory and density functional perturbation theory to characterize the inelastic relaxation mechanisms—phonon-phonon and electron-phonon interactions—that determine the lifetime of these phonon modes. We will discuss the relevance of these results to estimate the transport properties of carbon nanomaterials.

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Date submitted: 25 Nov 2008 Electronic form version 1.4