

Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Dielectric properties of carbon nanotubes from first principles¹

BORIS KOZINSKY, NICOLA MARZARI, Massachusetts Institute of Technology
— We characterize the response of single- (SWNT) and multi-wall (MWNT) carbon nanotubes to static electric fields using first-principles calculations and density-functional theory. The longitudinal polarizability of SWNTs scales as the inverse square of the band gap, while in MWNTs it is given by the sum of the polarizabilities of the constituent tubes. The transverse polarizability of SWNTs is insensitive to band gaps and chiralities and is proportional to the square of the effective radius; in MWNTs the outer few layers dominate the response. The transverse response is intermediate between metallic and insulating, and a simple electrostatic model based on a scale-invariance relation captures accurately the first-principles results. Dielectric response in both directions remains linear up to very high values of the applied field.

¹Supported by NSF/NIRT

Boris Kozinsky
Massachusetts Institute of Technology

Date submitted: 11 Jan 2006

Electronic form version 1.4