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Dielectric response of carbon and boron nitride nanotubes from first-principles calculations BORIS KOZINSKY, NICOLA MARZARI, Massachusetts Institute of Technology — We present a complete characterization of the dielectric response of isolated single- and multi-wall carbon (CNT) and boron-nitride nanotubes (BNNT) using first-principles calculations and density-functional theory. The longitudinal polarizability of a nanotube is sensitive to the band gap and its radius, and in multi-wall nanotubes and bundles it is trivially given by the sum of the polarizabilities of the constituent tubes. The transverse polarizability of both types of nanotubes is insensitive to band gap and chirality and depends only on the radius. However, the transverse response and screening properties of BNNTs are qualitatively different from those of metallic and semiconducting CNTs. The fundamental differences in electronic properties of the two materials are inherited from the corresponding two-dimensional sheets - graphene and boron-nitride. The screening of the external field in CNTs is stronger than in BNNTs and has a different radius dependence. The transverse response in BNNTs is found to be that of an insulator, while in CNTs it is intermediate between metallic and semiconducting. Our results have practical implications for selective growth of different types of nanotubes using aligning electric fields and for Raman characterization of nanotubes.

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