Dielectric properties of single-wall carbon nanotubes from first principles.

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We study the response of single-wall carbon nanotubes to static uniform electric fields. Polarizability tensors for metallic and semiconducting carbon nanotubes are computed using density-functional perturbation theory and compared to analytical predictions of the random phase approximation and classical electrostatics. We find that the longitudinal polarizability of semiconducting nanotubes is inversely proportional to the square of the band gap. The transverse polarizability, on the other hand, is independent of the gap and chirality of the nanotube of a given radius. These dependencies have practical implications for selective growth of different types of nanotubes using aligning fields as well as for methods of separating different kinds of nanotubes in solutions. In the regime of strong transverse electric fields we find a weak suppression of the gap in semiconducting nanotubes. We compare our results to earlier tight-binding calculations of polarizabilities as well as gap suppression.