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Chiral Dependent Optical Properties of Carbon Nanotubes

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We have carried out both empirical tight-binding (TB) and first-principles local-density functional (LDF) results for the electronic structure and predicted optical spectra of semiconducting single-walled carbon nanotubes (SWNT) for a range of diameters and chiralities. We have also carried out explicit calculations of the optical cross-sections for polarizations parallel and transverse to the nanotube axis. Recent photoluminescence experiments on these materials have been used to make assignments of the SWNT conformations based on tight-binding models for the excitation gap, E_{11}, between the van Hove singularities nearest the Fermi level, and the excitation gap, E_{22}, between the next set of van Hove singularities. Our results for the E_{11} and E_{22} gaps using these approaches show a strong dependence of the excitation spectra on the radius with a weak dependence on the chirality.. Although the TB and LDF results share similar dependence on the radius, the chirality dependence of the ratio E_{22}/E_{11} versus E_{22} differs substantially. We discuss and compare these results in light of other theoretical and experimental work on the optical properties of carbon nanotubes. This work was supported by the US Office of Naval Research, the DoD HPCMO CHSSI program through the Naval Research Laboratory, and Oklahoma State University.