# Covalent Functionalization of Single-Walled Carbon Nanotubes

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Carbon nanotubes play an important role in nanotechnology, including electronics, chemical sensors, and solar cells. Their electronic and optical properties are largely dependent on the chirality of the nanotube. Covalent functionalization is a way to further tune the electronic properties. The composition of these groups has been shown to affect the localization of the electron density and furthermore the emission and absorption energies and intensities. We hypothesize that the geometric placement of these groups, relative to the tube axis, is equally, if not more, important. Our goal is to be able to understand and predict band gap values and emission energies for any given functionalization and geometric positioning thereof. This will be achieved in three steps: (I) using density functional theory (DFT) calculations to obtain ground state structures, (II) examine band gap values and localization of electronic orbitals, (III) utilizing linear-response, time-dependent DFT to obtain the energy and intensity of optical transitions, which will provide further understanding of the effects of covalent functionalization on absorption and emission of CNTs.