# Effect of Chlorine Functionalization on Electronic and Optical Properties of Single-Walled Carbon Nanotubes

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Our research investigates the excited and ground state electronic properties of chlorinated single-walled carbon nanotubes (SWNT) using density functional theory (DFT) and time-dependent DFT (TDDFT) calculations. We performed calculations with both finite (6,2) tubes of different lengths and with applied periodic boundary conditions to determine the effect of methodology on the electronic structure of the SWNT. Different arrangements of two Cl ions or two neutral Cl atoms were compared. Negatively charged Cl ions adsorbed on the nanotube surface lead to a dramatic decrease in the band gap and the appearance of new states near the edge of the valence band (localized on and around the Cl ions) and conduction band (localized on the tube edges). This causes a major red shifting of the absorption spectra, with many optically dark or semi-dark lower energy transitions. However, the Cl ions have a relatively low binding energy, and are much less stable than neutral Cl atoms adsorbed on the nanotube surface. The neutral cases showed a much smaller decrease of the band gap; however, there was a substantial increase in the intensity of the lowest-energy optical transitions, and the Cl-nanotube interactions were relatively strong regardless of tube length.