# Predicting the Electronic Transport Properties of Chemically Functionalized Carbon Nanotubes: A Maximally Localized Wannier Function Approach

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Chemical functionalizations are one of the most promising routes to engineer the electronic properties of carbon nanotubes. While understanding the effect of various chemical groups is of fundamental interest, a full first-principles description on these complex nanostructures having thousands of atoms and randomly-distributed functional groups is still prohibitively expensive.

We calculate the quantum conductance of functionalized carbon nanotubes mapping first-principles calculations to tight-binding Hamiltonians built upon maximally localized Wannier function (MLWF) basis [1]. We apply this method to study two prototypical cases: monovalent and divalent functional groups, categorized according to the number of the covalent bonds that bind them to the nanotube backbone. One additional bond introduced by a monovalent group converts an $sp^2$ carbon to an $sp^3$ carbon on the sidewall. These $sp^3$ carbons strongly perturb the conduction $\pi$-manifold; a rapid decrease in the conductance is predicted as the number of the functional groups increases [1]. Divalent groups exhibit more interesting characteristic. The sidewall bond between the two neighboring carbon atoms associated with a functional group can either be broken or remain closed, which is determined by the curvature of the nanotubes and the chemical nature of the functional groups. Bond breaking transforms the two carbon atoms back to the $sp^2$ hybridized state; the conductance then approaches that of pristine nanotubes in contrast with the $sp^3$ hybridized case [2]. This theoretical prediction presents a novel concept of controlling the electronic transport of carbon nanotubes through an orbital rehybridization.

[1] Y.-S. Lee, M. Buongiorno Nardelli, and N. Marzari, Phys. Rev. Lett. **95**, 076804 (2005).

[2] Y.-S. Lee and N. Marzari, Phys. Rev. Lett. **97**, 116801 (2006).