Due to the exceptional strength, stiffness and excellent electrical and thermal properties, carbon nanotubes (CNTs) have been regarded as promising candidates for advanced nanoelectronics and multifunctional nanocomposites. In this dissertation, the interaction of CNTs with metals have been investigated and the resultant electrical conduction have been analyzed, aiming to develop innovative avenues to best utilize CNTs’ potential. In doing so, quantum mechanics calculations have been carried out to study obtain greater electrical conduction the possibility that doping metals (Cu, Al) could tailor the electronic three different types of metal-CNT interactions, 1) encapsulation of atoms inside the CNTs, 2) adsorption of atoms onto CNT surface, and 3) substitutional doping. Models of different doping methods were built and optimized with Density Functional Theory (DFT). And in conjunction with non-equilibrium Green’s function, the electronic structure and the conducting properties were calculated.

Through this study, both metal and semiconducting CNTs have been used. Metallic CNT (5, 5) encapsulated with copper chains have been first investigated with an emphasis on the electronic structure and the resultant conductance. The Density of States (DOS) have showed that the encapsulation of Cu effectively introduced more states around the fermi level. And due to the interaction between copper and CNTs, the conductance of the metallic CNTs-Cu system can be significantly increased.

In addition to copper, aluminum has been also introduced for the study. The electronic structure and transport properties of hybrid nanowires consisting of aluminum chains adsorbed on a single-wall semiconducting CNT (10, 0) have been calculated. The band structure and DOS of the hybrid nanowires have showed that the adsorption of Al can effectively reduce the band gap. And with more than 4 Al chains adsorbed, the CNTs have transformed from semiconducting to conducting. The transmission eigenstates further indicated that both Al chains and the modified nanotube were responsible for the increased conduction in the hybrid nanowires. The resultant conductance of CNT (10, 0)/Al hybrid nanowire is about 40% greater than that of pure Cu nanowire with the same diameter.

In order to utilize the extraordinary conductance in CNT(10,0)/Al hybrid nanowire, it is also important to investigate the end-contact between the hybrid nanowire with Al electrodes. During this work the transmission spectrum at different bias voltage were calculated to study the I-V characteristics and the electrical contact resistances at the interfaces. The results have suggested that the electrical contact resistances between Al electrodes and the hybrid nanowire is significantly lower than that of Al-pure CNT contacts, although the actual contact resistance is direction dependent that the contact resistance is reduced to 20% of that Al-pure CNT along the longitudinal direction.

The possibility of substitutional doping of Cu and Al in both metallic and semiconducting CNTs were also investigated. The formation energies have showed that Al doped was more energy favorable than Cu doping in both cases. And by doping of Al or Cu, a metallic tube experienced a higher conductance and a semiconducting tube has transited to conducting.
Approved for distribution by Quanfang Chen, Committee Chair, on October 17, 2016.

The public is welcome to attend.