Carbon nanotubes have been regarded as ideal building blocks for nanoelectronics and multifunctional nanocomposites due to their exceptional strength, stiffness, flexibility, as well as their excellent electrical properties. However, a carbon nanotube itself has limitations to fulfill the practical application needs: 1) an individual carbon nanotube has a low density of states at the Fermi level, and thus its conductivity is only comparable to moderate metals but lower than that of copper. 2) Metallic and semiconducting nanotubes are inherently mixed together from the synthesis, and the selection/separation is very difficult with very low efficiency. 3) Carbon nanotubes alone cannot be used in practical application and a bonding material is normally needed as the join material for actual devices.

In this work, we fundamentally explored the possibility that metals (Cu, Al) could tailor carbon nanotube’s electronic structure and even transit it from semiconducting to metallic, thus skipping the selection between the metallic and the semiconducting CNTs. We also found out a novel way to enhance a semiconducting CNT system’s conductance even better than that of a metallic CNT system. All these researches are done under density functional theory (DFT) frame in conjunction with non-equilibrium Green functions (NEGF).

At first we studied the adsorbed copper’s influence on the electronic properties of CNT (10, 0) and CNT (5, 5). Results indicate that both the Density of States (DOS) and the transmission coefficients of CNT (5,5)/Cu have been increased. For CNT(10,0)/Cu, the band gap has been shrunk, which means the improved conducting properties by the incorporation of copper.

As a further case, semiconductor SWCNT (10, 0) with more adsorbed copper chains outside has been studied. 1, 4, 5 and 6 Cu chains have been added onto the carbon nanotube (10,0), and the adsorption of 6 Cu chains finally lead to the transform of the system from semiconducting to metallic.

Considering the confining effect, the case that Cu filled into CNT (10,0) is also studied. It is found that the filled copper chains could modify the system to be metallic more efficiently than the adsorbed Cu chain.

Similarly, Al adsorbed on CNT(10, 0) is also studied, and it is found that Al has a better efficiency than copper in tuning the semiconducting CNT to metallic. The existing chemical bonds between the CNT and Al atoms may account for this higher efficiency. In addition, the resultant conductivity of the Al/CNT system is better than that of Cu/CNT system.

The Cu/CNT(5,5)+Cu/Cu junction, as another realistic device setup, has been studied in terms of the conductance. The results show that the incorporation of Cu would enhance the conductance of the Cu/CNT/Cu system due to the interaction between Cu and the CNT.
The public is welcome to attend.