MOLECULAR DOPING OF CARBON NANOTUBE NETWORKS

T. Ketolainen, V. Havu, E. Ö. Jónsson, and M. J. Puska

COMP, Department of Applied Physics, Aalto University, P.O. Box 11100,
FI-00076 Aalto, Finland
email: tomi.ketolainen@aalto.fi

The interest in carbon nanotube (CNT) thin films has increased remarkably during the recent years. These materials are expected to have numerous different applications including touch screens, solar cells, and light-emitting diodes [1]. A central problem with CNT thin films is to make a film that exhibits both high transparency and conductivity. Previous studies have shown that the conductivity of the CNT thin film can be improved by doping it with nitric acid [2]. Furthermore, it has been found computationally that $AuCl_4$ anions lead to a stable p-type doping effect [3].

The doping of single-walled metallic (8,8) and semiconducting (10,0) CNTs with $AuCl_4$ or NO_3 anions has been examined computationally in this work. We have used the FHI-aims code based on the density functional theory to compute band structures and electronic transmission functions for doped CNTs. In addition, electron transport in junctions of two perpendicular doped CNTs has been considered. Charge transfer from the CNT to the molecular anions is found in agreement with the recent study [3] and therefore the conductivity of doped semiconducting CNTs improves remarkably. Furthermore, adsorbed anions cause only little scattering. Junctions between doped CNTs show an enhanced intertube conductance because of the hybridization between CNT and molecular states. Due to the charge transfer from the CNT to the anion, the Fermi level is shifted down to a van Hove singularity. The large number of states at the Fermi level leads to the Fermi level pinning and good conductivity.

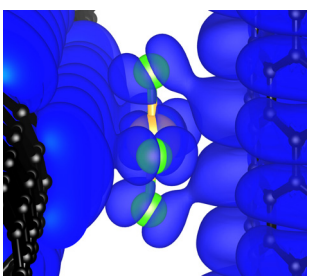

Figure 1: Hybridization between the orbitals of the $AuCl_4$ anion and the carbon atoms in a junction of two (10,0) CNTs.

[1] L. Yu, C. Shearer, and J. Shapter, Chem. Rev. **116**, 13413 (2016).
[2] W. Zhou, J. Vavro, N. M. Nemes, J. E. Fischer, F. Borondics, K. Kamarás, and D. B. Tanner, Phys. Rev. B **71**, 205423 (2005).
[3] A. Murat, I. Rungger, C. Jin, S. Sanvito, and U. Schwingenschlögl, J. Phys. Chem. C **118**, 3319 (2014).