Electron transport through functionalized carbon nanotubes

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KHALID ASHRAF, ROGER LAKE, University of California, Riverside — Single molecule functionalization of single walled carbon nanotubes (CNT)s by B. R. Goldsmith, et. al. [1] and single molecule bridges of single wall CNTs by X. Guo, et. al. [2] are elegant examples of CNT contacts to individual molecules for electronic applications. CNTs are of the same physical size as the molecule they contact providing a well-defined covalent bond between CNT electrodes and a molecule. The above two systems are studied to determine how a chemical absorbate and linker influence transport through metallic CNTs. The first system consists of a stand alone metallic CNT with a single oxygen adsorption site, matching a proposed final chemical process for a HNO$_3$ oxidation and reduction process. The second system consists of a CNT-Amide-(CH)$_n$-Amide-CNT structure in which both CNTs are metallic. Transmission calculations, using our DFT (FIREBALL)-NEGF code show that the amide linker suppresses transmission compared to a direct CNT-polyene linkage studied in [3]. 1. B. R. Goldsmith, et. al., Science, 315, 77 (2007). 2. X. Guo, et. al. Science, 311, 356 (2006). 3. N. Bruque, et. al. Phys. Rev. B, 76, 205322 (2007).