

Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Electron transport through functionalized carbon nanotubes

NICOLAS BRUQUE, RAJEEV PANDEY, University of California, Riverside, MD. 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 adsorbate 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).

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Date submitted: 05 Dec 2007

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