

Abstract Submitted
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Theory of the Conductance of a Single Molecule Connected to Metallic Single Wall Carbon Nanotube Electrodes¹ LEI ZHANG, YIING-REI CHEN, Chemistry Dept., Columbia University, MARK S. HYBERTSEN, Applied Physics and Applied Math Dept, Columbia University — Metallic single wall carbon nanotubes intuitively are expected to be ideal electrodes for making contact to small, conjugated organic molecules. In this work, the conductance of ideal junctions consisting of armchair nanotube electrodes connected by conjugated carbon chains is studied. A pi-electron tight binding model is used with a Greens function formulation of the electronic states in the junction and the conductance. Key factors that influence the conductance of these junctions include molecule length, electrode attachment topology, and even versus odd length. This study delimits the maximum conductance that can be ideally expected using metallic nanotube electrodes.

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Mark S. Hybertsen
Applied Physics and Applied Math Dept, Columbia University

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