Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

First-Principles electronic transport calculations in finite elongated systems: A divide and conquer approach[1] ODED HOD, JUAN E. PERALTA, GUSTAVO E. SCUSERIA, Department of Chemistry, Rice University, Houston, Texas 77005 — We present a *first-principles* method for the evaluation of the transmittance probability and the coherent conductance through *finite-elongated* systems composed of a repeating molecular unit and terminated at both ends. Our method is based on a divide and conquer approach in which the Hamiltonian of the elongated system can be represented by a block tridiagonal matrix, and therefore can be readily inverted. This allows us to evaluate the transmittance and the conductance using first-principles electronic structure methods without explicitly dealing with calculations involving the entire system. A proof of concept model based on a *trans*-polyacetylene chain bridging two aluminum leads indicates that our divide and conquer approach is able to capture all of the features appearing in the transmittance probability curves of a full scale calculation. Using our method we investigate the edge effects on the electronic structure of finite sized carbon nanotubes as a function of their length and identify the limit at which the electronic structure converges to that of an infinite system.

[1]This research was supported by the National Science Foundation under Grant CHE-0457030. O.H. would like to thank the generous financial support of the Rothschild and Fulbright foundations.

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Date submitted: 06 Dec 2006 Electronic form version 1.4