

Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Electron Propagator Calculations on Molecular Wires. J.V. ORTIZ, V.G. ZAKRZEWSKI, Department of Chemistry, Kansas State University, 111 Willard Hall, Manhattan, KS 66506-3701, ALEXEY KLETSOV, Department of Electrical Engineering, University of Wyoming, 1000 E. University Avenue, Laramie, WY 82071, YURI DAHNOVSKY, Department of Physics & Astronomy/3905, University of Wyoming, 1000 E. University Avenue, Laramie, WY 82071, J. V. ORTIZ AND V. G. ZAKRZEWSKI COLLABORATION, YURI DAHNOVSKY AND ALEXEY KLETSOV COLLABORATION — Several molecular wires are studied by an *electron propagator* method using a non-self-consistent formalism for the calculation of Keldysh functions. This approach is based on diagrammatic approximations for describing electron correlation in a bridge molecule that have been successful in the *ab initio* determination of electron binding energies. In this work, we compute nonequilibrium Keldysh functions in order to find the dependence of current on applied voltage for particular molecular wires. Quantum chemical calculations are performed for several molecular bridges and require additional computational method development of established electron propagator techniques. The extended molecule approach is adopted. Results are compared with experimental data and other quantum chemical approaches, especially those based on density functional theory.

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Date submitted: 16 Sep 2005

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