Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Molecular conductance simulations with a 'hybrid' DFT-NEGF approach ALEXANDER PROCIUK, BARRY DUNIETZ, University of Michigan — A time propagated DFT-NEGF methodology for describing molecular conductance through extended metal-molecule-metal systems is developed. This innovative method calculates transient currents in the presence of time dependent perturbations applied to the molecular junction. Steady state currents can be calculated in the presence of finite temporal perturbations. The electronic density, represented by the lesser GF, is recast into a form that expresses the temporal propagation of the energy spectrum. The effects of the potential biased metal electrodes are expressed with energy dependent 'self-energy' terms. This results in a manageable and compact expression for the electron density. This density can be propagated by a specialized scheme that elucidates the transport properties of the system. Propagation, in the absence of an applied temporal perturbation, reduces to an alternative and novel NEGF transport methodology. In addition, applied perturbations can be propagated fully or approximated to any order in time dependent perturbation theory. Calculations are performed for various DFT functionals with a LANL2DZ ECP basis set.

Alexander Prociuk
University of Michigan

Date submitted: 21 Nov 2006 Electronic form version 1.4