Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Time dependent transport in nanostructures[1] KALMAN VARGA, Vanderbilt University — Using the Lagrange-function representation [1] we present time-dependent density functional calculations of the transport properties of nanostructures. To avoid the complications related to the semiinfinite leads a complex absorbing potential (CAP) is added to the Hamiltonian [2,3]. This transformation leads to an effectively closed system which is computationally manageable. We will compare the results of the time dependent approach to those of time independent approaches for prototypical molecular devices such as benzene ring between gold electrodes and nanotubes.

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[1]Supported by NSF ECS 0622146.

Kalman Varga
Vanderbilt University

Date submitted: 20 Nov 2008 Electronic form version 1.4