Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Open Quantum Transport and Non-Hermitian Real-Time Time-Dependent Density Functional Theory JUSTIN ELENEWSKI, Department of Chemistry, The George Washington University, YANXIANG ZHAO, Department of Mathematics, The George Washington University, HANNING CHEN, Department of Chemistry, The George Washington University — Sub-nanometer electronic devices are notoriously difficult to simulate, with the most widely adopted transport schemes predicting currents that diverge from experiment by several orders of magnitude. This deviation arises from numerous factors, including the inability of these methods to accommodate dynamic processes such as charge reorganization. A promising alternative entails the direct propagation of an electronic structure calculation, as exemplified by real-time time-dependent density functional theory (RT-TDDFT). Unfortunately this framework is inherently that of a closed system, and modifications must be made to handle incoming and outgoing particle fluxes. To this end, we establish a formal correspondence between the quantum master equation for an open, many-particle system and its description in terms of RT-TDDFT and non-Hermitian boundary potentials. By dynamically constraining the particle density within the boundary regions corresponding to the device leads, a simulation may be selectively converged to the non-equilibrium steady state associated with a given electrostatic bias. Our numerical tests demonstrate that this algorithm is both highly stable and readily integrated into existing electronic structure frameworks

Justin Elenewski
Department of Chemistry, The George Washington University

Date submitted: 06 Nov 2015 Electronic form version 1.4