Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

First-principles parameter-free calculations of electron mobilities in silicon: phonon and Coulomb scattering OSCAR D. RESTREPO, KALMAN VARGA, Vanderbilt University, SOKRATES T. PANTELIDES, Vanderbilt University and ORNL — Mobility is a key factor in charge transport since it describes how the motion of an electron is affected by an applied electric field. As such, it is an important element in the design of new devices. Mobilities are generally modeled using methods that suppress atomic-scale detail (effective mass theory or bulk energy bands for electron velocities, empirical deformation potentials, macroscopic roughness, etc). Parameter fitting to experimental data is needed. As new technologies require modeling of transport at the nanoscale and new materials are introduced, predictive parameter-free mobility modeling is needed. The main scattering mechanisms that limit mobilities are due to phonon, ionized impurities, and interface roughness. A first-principles calculation of mobilities limited by atomic scale roughness with atomic-scale detail was reported recently [1]. We report the development of parameter-free quantum-mechanical methods to calculate scattering rates and electron mobilities limited by phonon and ionized-impurity scattering in a self-consistent way. Results for n-doped silicon are in good agreement with experimental data. This work was supported by NSF Grant ECS-0524655. [1] M. H. Evans et al., Phys. Rev. Lett. 95, 106802 (2005).

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Date submitted: 10 Dec 2008 Electronic form version 1.4