Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Density functional calculations of multiphonon capture cross sections at defects in semiconductors[1] GEORGIOS D. BARMPARIS, YEVGENIY S. PUZYREV, Vanderbilt University, X.-G. ZHANG, Oak Ridge National Laboratory, SOKRATES T. PANTELIDES, Vanderbilt University — The theory of electron capture cross sections by multiphonon processes in semiconductors has a long and controversial history. Here we present a comprehensive theory and describe its implementation for realistic calculations. The Born-Oppenheimer and the Frank-Condon approximations are employed. The transition probability of an incoming electron is written as a product of an instantaneous electronic transition in the initial defect configuration and the line shape function (LSF) that describes the multiphonon processes that lead to lattice relaxation. The electronic matrix elements are calculated using the Projector Augmented Wave (PAW) method which yields the true wave functions while still employing a plane-wave basis. The LSF is calculated by employing a Monte Carlo method and the real phonon modes of the defect, calculated using density functional theory in the PAW scheme. Initial results of the capture cross section for a prototype system, namely a triply hydrogenated vacancy in Si are presented. The results are relevant for modeling device degradation by hot electron effects.

[1]This work is supported in part by the Samsung Advanced Institute of Technology (SAIT)'s Global Research Outreach (GRO) Program and by the LDRD program at ORNL.

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Date submitted: 14 Nov 2013 Electronic form version 1.4