Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Nonradiative hot carrier capture cross section of defects in GaN from first principles[1] JUN JIANG, Department of Physics and the Quantum Theory Project, University of Florida, Gainesville, Florida, GEORGIOS D. BARMPARIS, Crete Center for Quantum Complexity and Nanotechnology, Department of Physics, University of Crete, Heraklin, Greece, SOKRATES T. PANTELIDES, Department of Electrical Engineering and Computer Science, Vanderbilt University, Nashville, Tennessee, X.-G. ZHANG, Department of Physics and the Quantum Theory Project, University of Florida, Gainesville, Florida — Recent progress in first-principles calculations of multiphonon processes in solids [1,2] allows direct calculation of nonradiative hot-carrier capture cross sections of defects in semiconductors. We apply the computational method in [1] to electron and hole capture cross sections of defects in GaN. As formulated, the method contains zeroth-order matrix elements for the phonon-assisted electron (or hole) transition, whose contribution is expected to be larger than the contributions of the usual, first-order, electron-phonon coupling matrix elements [2]. The calculated cross sections are compared to the first-order results in [2] and to experiments. [1] Barmparis, Georgios D., et al. Physical Review B 92.21 (2015): 214111. [2] Alkauskas, A., et. al, Physical Review B, 90(7), 075202.

[1]Acknowledgments: NSF grant ECCS-1508898

Jun Jiang
Univ of Florida - Gainesville

Date submitted: 11 Nov 2016 Electronic form version 1.4