Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

First-principles theory of radiative and nonradiative carrier capture rates at defects in semiconductors[1] AUDRIUS ALKAUSKAS, CYRUS E. DREYER, JOHN L. LYONS, QIMIN YAN, CHRIS G. VAN DE WALLE, University of California Santa Barbara — We have developed a first-principles approach to calculate radiative and nonradiative carrier capture coefficients (cross sections) at defects in semiconductors. The methodology is based on the use of hybrid density functionals that provide an excellent description of both bulk and defect properties. As test cases, we applied the methodology to selected defects in GaN and ZnO. We have obtained excellent agreement with experimental results in the few cases where they are available. For deep acceptors, radiative electron capture cross sections are of the order 10^{-5} Å^2, while nonradiative hole capture cross sections are in the range 1-500 Å^2. Our results will (i) be very helpful for identifying the microscopic origin of defects in GaN and ZnO; (ii) provide fundamental insights into the origin of traps in electronic devices based on these materials; and (iii) help finding and controlling the centers responsible for Shockley-Read-Hall recombination in nitride optoelectronic devices. This work was supported by DOE.

[1]This work was supported by DOE.

Audrius Alkauskas
University of California Santa Barbara

Date submitted: 14 Nov 2013 Electronic form version 1.4