Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Nonradiative carrier capture rates at defects from first-principles calculations QIMIN YAN, AUDRIUS ALKAUSKAS, CHRIS G. VAN DE WALLE, Materials Department, University of California at Santa Barbara — We develop a computational methodology to determine nonradiative carrier capture rates at defects in wide-band-gap semiconductors. In our theoretical framework, we consider carrier capture via multiphonon emission as the dominant nonradiative mechanism for deep defects in wide-band-gap materials at low and moderate carrier densities. Our methodology is based on the static approximation for the electron-phonon coupling. We employ a state-of-the-art hybrid density functional approach to describe the electronic structure. For charged defect systems, the screening effect by excess carriers is taken into account. As test cases, we investigate deep centers including C_N and V_{Ga} in GaN and Li_{Zn} in ZnO. Calculated carrier capture rates are in good agreement with available experimental data. This work was supported by DOE, NSF, Swiss NSF, and by the UCSB SSLEC.

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Date submitted: 09 Nov 2012 Electronic form version 1.4