Abstract Submitted for the MAR13 Meeting of The American Physical Society

Phonon-Assisted Auger Recombination in Gallium Arsenide and Gallium Nitride from First Principles<sup>1</sup> DANIEL STEIAUF, Materials Department, University of California, Santa Barbara, EMMANOUIL KIOUPAKIS, Materials Science and Engineering, University of Michigan, Ann Arbor, CHRIS G. VAN DE WALLE, Materials Department, University of California, Santa Barbara — GaN and GaAs and their alloys are technologically important materials for solidstate optoelectronic devices such as light emitting diodes. The internal quantum efficiency of these devices, defined as the fraction of electron-hole pairs converted to photons, is limited by non-radiative loss mechanisms. Auger recombination is such a mechanism which decreases the efficiency at high current densities. In this process, the energy and momentum of an electron-hole pair is transferred to a third carrier. Numerically it is found that this process does not lead to relevant loss rates. However, if a phonon is emitted or absorbed at the same time, Auger loss rates increase by several orders of magnitude. We calculate the Auger recombination rate coefficients from first principles using density functional theory. Treating also the phonons from first principles allows us to analyze which modes and wave vectors contribute predominantly to Auger recombination and the non-radiative loss in these materials.

<sup>1</sup>This work was supported by DOE.

Daniel Steiauf Materials Department, University of California, Santa Barbara

Date submitted: 09 Nov 2012

Electronic form version 1.4