Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Vibrational structure of defect luminescence bands in GaN from electronic structure calculations AUDRIUS ALKAUSKAS, CHRIS G. VAN DE WALLE, Materials Department, University of California Santa Barbara, CA 93106-5050 — Optical methods are among the most powerful to characterize defects in materials. The study of optical signatures based on state-of-the-art electronic structure methods is therefore very important. In this work we investigate the vibrational structure of luminescence bands pertaining to deep defect levels in GaN. Since luminescence lineshapes depend sensitively on defect geometries and vibrational frequencies, these should be described accurately. The latter is achieved through the use of hybrid density functionals. Both quasi-localized and bulk phonons are included in our description. In the case of transitions accompanied by very large lattice relaxations, anharmonic effects become sizeable, and these are also accounted for. For the defects studied a very good agreement with available experimental data is achieved. For instance, in the case of wide luminescence bands the resulting line widths are within 0.05 eV of the experimental values. This work was supported by the Swiss NSF and by NSF.

Audrius Alkauskas
Materials Dept, University of California Santa Barbara, CA 93106-5050

Date submitted: 28 Nov 2011 Electronic form version 1.4