Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Temperature-dependence of electron bands in wurtzite GaN, including non-adiabatic (Polaron) contributions[1] JEAN PAUL NERY, JIAN LIU, P. B. ALLEN, Stony Brook University — We study the temperature dependence of the band gap of wurtzite structure GaN [1]. Virtual interband electron-phonon scattering is accounted properly by adiabatic (Allen-Heine-Cardona) theory. The correct way to avoid an unphysical divergence, is to use a non-adiabatic treatment for intraband scattering by small q polar optical phonons [2,3]. This is equivalent to including Fröhlich polaron effects. The $T = 0$ zero-point weak-coupling polaron shift ($-\alpha\hbar\omega$) is well known, but finite T effects are less studied. We also calculate the T dependence of the band mass (both polaron and adiabatic contributions). We compare results from an *ab-initio* density-functional approach with those obtained starting from the traditional Fröhlich Hamiltonian approach. [1] M. Cardona and Kremer, Thin Solid Films **571**, 680 (2014). [2] S. Poncé *et al.*, The Journal of Chemical Physics **143**, 102813 (2015) [3] C. Verdi and F. Giustino, Phys. Rev. Lett. **115**, 176401 (2015)

[1]Supported in part by DOE grant No. DE-FG02-08ER46550.

Jean Paul Nery
Stony Brook University

Date submitted: 06 Nov 2015 Electronic form version 1.4