Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Ab Initio Calculations of Excited Carrier Dynamics in Gallium Nitride VATSAL JHALANI, MARCO BERNARDI, California Institute of Technology — Bulk wurtzite GaN is the primary material for blue light-emission technology. The radiative processes in GaN are regulated by the dynamics of excited (or so-called hot) carriers, through microscopic processes not yet completely understood. We present ab initio calculations of electron-phonon (e-ph) scattering rates for hot carriers in GaN. Our work combines density functional theory to compute the electronic states, and density functional perturbation theory to obtain the phonon dispersions and e-ph coupling matrix elements. These quantities are interpolated on fine Brillouin zone grids with maximally localized Wannier functions, to converge the e-ph scattering rates within 5 eV of the band edges. We resolve the contribution of the different phonon modes to the total scattering rate, and study the impact on the relaxation times of the long-range Fröhlich interaction due to the longitudinal-optical phonon modes.

Vatsal Jhalani
Caltech

Date submitted: 02 Nov 2015 Electronic form version 1.4