



MATERIALS DEPARTMENT / MRL  
JOINT COLLOQUIUM

Friday, October 16, 2009, 4:00 PM, ESB 1001



# “Theoretical Spectroscopy - getting to know your favorite group-III-nitride”

## Dr. Patrick Rinke

Postdoctoral Scholar  
Materials Department  
University of California, Santa Barbara

### Abstract

The group-III-nitrides (Al,Ga,In)N and their alloys are currently the only commercially available materials class for the green to ultraviolet part of the spectrum in optoelectronic devices. The market for light emitting devices (LED) and laser diodes has grown extensively in the last few years and nitride-based photovoltaic solutions for clean energy generation are being explored. Solid state lighting is already rivaling incandescent and fluorescent light sources, but to decrease the cost an increase in internal quantum efficiency is required. In light of this tremendous research effort it is therefore surprising that many open questions regarding the characterization and fundamental understanding of the group-III-nitrides remain, whose resolution would significantly expedite progress in device design. This is the domain of theoretical spectroscopy - the domain of quantum mechanical calculations of elementary excitations on the atomic scale.

In this talk I will demonstrate that rigorous first-principles calculations can fill this gap. By combining density functional theory for the atomic structure with many-body perturbation theory in the  $G_0W_0$  approximation for the quasiparticle band structure we achieve an accurate and consistent description of the bulk phases of AlN, GaN and InN at the equilibrium volume and under strain [1,2,3]. Building on this we investigate individual loss mechanisms, that are difficult to detect and disentangle experimentally, but can easily be isolated in theoretical calculations. Auger recombination (a three particle scattering process) has been proposed by Shen *et al.* [4] to explain the "droop", the efficiency loss at high drive currents, in nitride-based light emitters.

We show that Auger recombination is a key loss mechanism in wurtzite InGaN in the blue to green spectral region and becomes an important non-radiative loss mechanism at high current densities, since it scales with the cubic power of the free-carrier concentration [5]. To study direct and phonon-assisted absorption of light by free carriers in the nitrides we have developed a first-principles formalism that efficiently combines density functional and many-body perturbation theory. We find that the free-carrier absorption spectrum of GaN in the visible is dominated by phonon-assisted processes and that free-carrier absorption is a relevant loss mechanism in nitride light emitters, in particular for laser devices operating at longer wavelengths [6].

[1] P. Rinke *et al.*, Phys. Rev. B 77, 075202 (2008).

[2] P. Rinke *et al.*, Appl. Phys. Lett. 89, 161919 (2006).

[3] Q. Yan, P. Rinke, M. Scheer and C. G. Van de Walle, Appl. Phys. Lett. 95, 121111 (2009).

[4] Y. C. Shen *et al.*, Appl. Phys. Lett. 91, 141101 (2007).

[5] K. T. Delaney, P. Rinke, and C. G. Van de Walle, Appl. Phys. Lett. 94, 191109 (2009).

[6] E. Kioupakis *et al.*, Phys. Rev. Lett. submitted.

Host: Professor Chris Van de Walle

**LIGHT REFRESHMENTS WILL BE SERVED PRIOR TO THE SEMINAR AT 3:45PM**