

### TRR Guest Scientist Lecture / Seminar

Date/Time: 08.06.2016 / 4 pm

Location: Paderborn / Lecture Hall A1

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## Electronic and optical properties of nitride-based heterostructures: carrier localization effects in wurtzite InGaN and InAlN systems

#### Abstract:

The electronic and optical properties of InAlN and InGaN systems are of interest for a variety of different applications. However, key material parameters are still not well understood. For instance, a large degree of uncertainty in the band gap bowing parameters has been reported in the literature and even composition dependent bowing parameters have been suggested. This question is not only from a fundamental material property perspective of interests, also for device design the band variation with indium content is of central importance. Furthermore, experimental studies clearly show that electronic and optical properties of III-N alloys are in general significantly affected by random alloy fluctuations present in these systems. An example is the unusual defect insensitivity found in (In,Ga,Al)N alloys, which has been imputed to localization of carriers due to alloy fluctuations. Nevertheless, theoretical studies of nitride-based heterostructures have focused mainly on continuum based descriptions, which do not capture fully the effects introduced by fluctuations on an atomic scale.

We present here an atomistic analysis of wave function localization effects in InAlN alloys and InGaN quantum wells (QWs) with random indium distributions and structural inhomogeneities, such as well-width fluctuations. The InGaN QW structures studied range from standard *c*-plane structures to nonpolar *m*-plane systems. We show here that the local indium configurations strongly affect the conduction band edge wave function in InAlN alloys with low indium contents (cf. Fig. 1), while the valence band edge state becomes increasingly localized as an increasing number of indium atoms share a N atom in InAlN alloys and in InGaN QW structures. Furthermore, our results on nonpolar *m*-plane QW samples are compared in detail with (time-dependent) photoluminescence experiments, revealing for instance strong exciton localization effects, which explain the form of the measured photoluminescence decay transients. Additionally, the theoretical results confirm the experimentally observed high degree of optical linear polarization. Overall, we conclude that random alloy fluctuations have a critical impact on the electronic structure of InAlN and InGaN systems, and consequently affect their optical properties significantly. Our results also show that these fluctuations are best assessed using atomistic approaches.

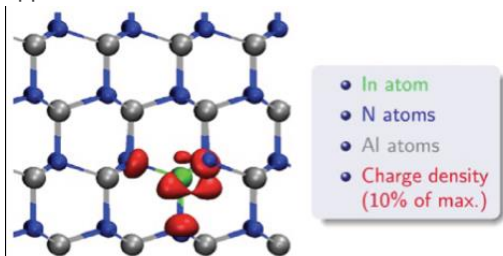


Fig. 1: Indium related localized state in AlInN

This seminar was jointly organized by the SFB TRR142 and the GRK1464

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