Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Doping and defects in AlN and InN[1] CHRIS VAN DE WALLE, Materials Department, University of California, Santa Barbara — First-principles calculations have significantly contributed to our understanding of defects and impurities in GaN. Here I will present new results for AlN and InN. UV light emitters require AlGaN alloys with high Al content, in which doping becomes increasingly problematic. In addition, bulk AlN is being considered as a substrate material, prompting an investigation of the origin of various absorption lines. For n-type doping, DX-center formation turns shallow impurities such as O, Si, or Ge into deep centers. I will present detailed configuration-coordinate diagrams that summarize the prospects of using these impurities for doping. Al vacancies, as well as their complexes with oxygen, can also occur, and I will discuss specific proposals for the optical absorption lines typically observed at 2.8 eV and 4.5 eV. Turning to InN, a major challenge is to control the n-type conductivity observed in nominally undoped material. Calculations show that point defects such as nitrogen vacancies are unlikely to be responsible for this unintentional conductivity. It is more plausibly caused by impurities such as oxygen. In the case of InN we have found that an even more common impurity can act as a shallow donor, namely hydrogen. Detailed results for the atomic and electronic structure of hydrogen in various configurations will be discussed.

[1]This work was supported in part by ONR and AFOSR.

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Date submitted: 30 Nov 2004 Electronic form version 1.4