

Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Role and Effect of Native Defect Complexes in InN XIANGMEI DUAN, CATHY STAMPFL, School of Physics, The University of Sdney, CONDENSED MATTER THEORY TEAM — We have carried out the first-principles density-functional theory calculations to investigate the structural and electronic properties and the formation energies of native point defect complexes in InN. We report an extensive and systematic study of possible configurations and different concentrations, focusing on the nitrogen- and indium-vacancies. Nitrogen vacancies prefer to be situated close to one another resulting in local metallic indium-rich regions or “clustering”; while indium vacancies prefer to be separated, or to cluster together, where neighbouring under-coordinated N atoms spontaneously form N₂ molecules. These defect structures induce marked changes in the states in the region of the band gap, which may explain the wide variation in experimentally determined band-gaps (see e.g. [1]).

[1] T. V. Shubina, et al. Phys. Stat. Sol. (a) 202, 377 (2005).

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Date submitted: 28 Nov 2005

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