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**Effect of Native Defects in InN: Metallic bonding and N<sub>2</sub> Formation** XIANGMEI DUAN, CATHERINE STAMPFL, School of Physics, The University of Sydney, Australia — Despite intense investigations, development of indium nitride technology remains at the stage of seeking to improve the growth techniques and fabrication of device-quality material. Doping and impurity control is essential for the advancement of InN-based electronic and optoelectronic devices, yet even the role of native point defects in InN, and their effect on the physical and electronic properties, is still lacking [1]. We have thoroughly investigated the distribution and electronic properties of native point defects in wurtzite InN through first-principles density-functional theory calculations. We find that both the nitrogen and indium vacancies have a tendency to form “clusters” in the neutral and negative charge states. For nitrogen vacancies, this results in local indium-rich regions with metallic-like bonds, while we find molecular nitrogen formation occurs either by the clustering of indium vacancies, or interstitial nitrogen. The formation energies of the indium vacancy clusters are however rather high, but that of interstitial nitrogen in the 3+ charge state has a low formation energy under N-rich conditions. Our results help to explain a number of hitherto puzzling experimental observations[1-3]. [1] T. Shubina et al. Phys. Stat. Sol. a **202**, 377 (2005). [2] Y. Davydov et al. Phys. Stat. Sol. B **230**, R4(2002); **240**, 425 (2003). [3] H. Timmers et al. J. Cryst. Growth **288**, 236 (2006).

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