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The role of nitrogen vacancies and hydrogen in conductivity of InN ANDERSON JANOTTI, CHRIS G. VAN DE WALLE, Materials Department, University of California, Santa Barbara, CA 93106 — Using first-principles methods we investigate the electronic properties and stability of the nitrogen vacancy and monatomic hydrogen in InN. We find that nitrogen vacancies act as shallow donors, but they have high formation energies in n-type InN. Therefore, N vacancies are unlikely to cause the observed unintentional n-type conductivity in as-grown InN. Hydrogen can occupy interstitial as well as substitutional sites in InN. Interstitial hydrogen has low formation energy, is stable in the bond-center configuration, and acts exclusively as a shallow donor (H_i^+). The calculated frequency of the H-N stretching mode is 3050 cm^{-1}. Hydrogen can also substitute for nitrogen in InN, bonding equally to the four In nearest neighbors in a multicenter-bond configuration [1]. Substitutional hydrogen also has low formation energy and, counterintuitively, forms a double-donor center. Our results suggest that monatomic hydrogen is a plausible cause of the unintentional n-type conductivity that is almost universally observed in as-grown InN.
[1] A. Janotti and C. G. Van de Walle, Nature Mater. **6**, 44 (2007).

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