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N-H vibrational frequencies in GaAs:N:H$_n$ W. BEALL FOWLER, M. STAVOLA, LANLIN WEN, Lehigh University, A. POLIMENI, M. CAPIZZI, University of Rome — While the fundamental H-related defect in GaAs:N and GaP:N appears to have an NH_2 character,[1] considerable recent evidence suggests that an additional one or two hydrogen atoms may in some cases be involved.[2,3] We have used the CRYSTAL06 *ab initio* quantum code[4] with density functional theory to investigate these possibilities, obtaining theoretical equilibrium positions, ground-state energies, and vibrational frequencies with all combinations of H and D. In all cases investigated, the NH_2 configuration is preserved, but observable shifts in the N-H or N-D vibrational frequencies are predicted. Supported by NSF Grant 541744. [1] S. Kleekajai *et al.,* Phys. Rev. B **77**, 085213 (2008) and references contained therein. [2] A. A. Bonapasta *et al.*, Phys. Rev. Lett. **98**, 206403 (2007). [3] M. Berti *et al.*, Phys. Rev. B **76**, 205323 (2007). [4] R. Dovesi *et al.*, *Crystal06 User's Manual* (University of Torino, Torino, 2006).

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