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Structure and local vibrational frequencies of the 2H complex in H-irradiated GaAs:N MAO-HUA DU, SUKIT LIMPIJUMNONG, SHENG-BAI ZHANG, National Renewable Energy Laboratory — Hydrogen irradiation of GaAs:N samples leads to a giant blue shift of the band-gap [1]. Insight on the H complex has recently been available through infrared studies [2], showing three distinct H-modes (3195, 2967, and 1447 cm^{-1}), all correspond to N-H bonds. The absence of the Ga-H bond, however, contradicts previously proposed low-energy H_2* model where one H is on Ga whereas the other is on N [3]. Analysis of the measured isotope shifts shows that the H complex in the H-irradiated GaAs:N samples should involve two coupled H atoms. Based on density functional calculations, we propose a new nitrogen-2H complex. Not only the model accounts for the observed giant blue shift due to H-irradiation, but the calculated H-vibrational frequencies (3207, 3052, and 1417 cm^{-1}) and isotope shifts are also in good agreement with experiment. Supported by the U. S. DOE/ BES and EERE under contract No. DE-AC36-99GO10337. [1] G. Baldassarri H. v. H., et al., Appl. Phys. Lett.**78**, 3472 (2001) [2] F. Jiang, et al., Phys. Rev. B **66**, 073313 (2002) [3] A. Janotti, et al. Phys. Rev. Lett. **89**, 086403 (2002)

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