

Abstract Submitted  
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**Ab-initio study of dilute nitride substitutional and split-interstitial impurities in gallium antimonide (N-GaSb)<sup>1</sup>** PRIYAMVADA JADAUN, HARI P. NAIR, SETH R. BANK, SANJAY K. BANERJEE, The University of Texas at Austin — We present an ab-initio density functional theory study of dilute-nitride GaSb. Adding dilute quantities of nitrogen causes rapid reduction in bandgap of GaSb ( $\sim 300$  meV for 2% N). Due to this rapid reduction in bandgap, dilute-nitrides provide a pathway for extending the emission of GaSb based type-I diode lasers into the mid-infrared wavelength region (3-5 micron). In this study we look at the effect of substitutional N impurity on the electronic properties of our system and compare it with the band-anticrossing model, a phenomenological model, which has been used to explain giant band bowing observed in dilute-nitride alloys. We also study the effect of Sb-N split interstitials which are known to be non-radiative recombination centers. Furthermore we also discuss the stability of the Sb-N split interstitial relative to substitutional nitrogen to determine if the split interstitials can be annihilated using post-growth annealing to improve the radiative lifetime of the material which essential for laser operation.

<sup>1</sup>NSF Teragrid machine Ranger at Texas Advanced Computing Center.

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