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Electronic and optical properties of GaSb:N from first principles[1]
PRIYAMVADA JADAUN, HARI NAIR, Cornell University, VINCENZO LORDI, Lawrence Livermore National Laboratory, SETH BANK, SANJAY BANERJEE, University of Texas at Austin — We present an ab-initio study of dilute nitride III-Vs, focusing on dilute nitride GaSb (GaSb:N). GaSb:N displays promise towards realization of optoelectronic devices accessing the mid-infrared wavelength regime. Theoretical and experimental results on its electronic and optical properties are however few. To address this, we present a first principles, density functional theory study using the hybrid HSE06 exchange-correlation functional of GaSb doped with 1.6% nitrogen. We conduct a comparative study on GaAs:N, also with 1.6% nitrogen mole fraction, and find that GaSb:N has a smaller band gap and displays more band gap bowing than GaAs:N. In addition we examine the orbital character of the bands, finding the lowest conduction band to be quasi-delocalized, with a large N-3s contribution. At high concentrations, the N atoms interact via the host matrix, forming a dispersive band of their own which governs optoelectronic properties and dominates band gap bowing. While this band drives the optical and electronic properties of GaSb:N, its physics is not captured by traditional models for dilute-nitrides. We thus propose that a complete theory of dilute-nitrides should incorporate orbital character examination, especially at high N concentrations.

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