Abstract Submitted
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Understanding the Impact of Point Defects on the Optoelectronic Properties of Gallium Nitride from First-Principles[1] KIRK LEWIS, MASAHIKO MATSUBARA, ENRICO BELLOTTI, SAHAR SHARIFZADEH, Department of Electrical and Computer Engineering, Boston University — Gallium nitride (GaN) and related alloys form a class of wide bandgap semiconductors that have broad applications as components in optoelectronic devices; in particular, power electronics and blue and ultraviolet optical devices. Nitride films grow with high defect densities, and understanding the relationship between structural defects and optoelectronic function will be central to the design of new high-performance materials. Here, we take a first-principles density functional theory (DFT) and many-body perturbation theory (MBPT) approach to quantify the influence of defects on the electronic and optical properties of GaN. We predict, as expected, that introduction of a N or Ga vacancy results in several energetically favorable charged states within bulk GaN; these energetically favorable defects result in a significant modification of the quasiparticle and excitonic properties of GaN. We will discuss the implications of defect-induced-states for the electron transport and absorption properties of GaN.

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