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Optoelectronic Properties of Point Defects in Gallium Nitride: A Many-Body Perturbation Theory Perspective[1] KIRK LEWIS, SAHAR SHARIFZADEH, Boston University — Gallium nitride (GaN) and related alloys form a class of wide bandgap semiconductors that have broad applications in optoelectronics technology such as blue/ultraviolet optical devices and power electronics. However, these materials generally grow with high defect densities, which can substantially degrade their optical and electronic properties. An accurate and detailed knowledge of the influence of defects on the optoelectronic properties of these materials is central to the design of new high-performance materials. We employ first-principles many-body perturbation theory within the GW/BSE approximation to investigate the influence of defects on the optical and electronic properties of bulk GaN, taking the nitrogen vacancy as an example. GW calculations predict that introduction of the vacancy results in significant modification of the electronic properties of GaN due to the presence of shallow trap states, an effect that is partially captured by standard DFT. Additionally, we predict strong exciton binding energies associated with excitations near defects. Our analysis suggests that it is necessary to go beyond standard DFT to understand excited-states near shallow defects.

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