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First Principles Green's Function Calculations of the Electronic and Optical Properties of Point Defects in GaN SOHRAB ISMAIL-BEIGI, Yale University — Despite the successful use of GaN in light-emitting and laser diodes, its materials properties are not well understood or controlled: typical samples have high densities of point and extended defects. A wealth of experimental information exists on these defects, but disentangling the contributions of individual defects from aggregated measured signals requires theoretical input. To date, first principles studies of these defects have used density functional theory (DFT) to study their formation energies, charge states, and structures. However, DFT provides poor predictions of electronic excitations and thus optical and luminescence properties, whereas many experiments probe these very properties. We apply state-of-the-art first principles Green's functions methods (based on the GW approximation and the Bethe-Salpeter Equation) to GaN point defects. These methods have proven accurate enough to provide direct comparisons to experiments for a variety of materials. We report mainly on the properties of the gallium and nitrogen vacancies, V_{Ga} and V_N, native defects with favorable formation energies in typical GaN samples.

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