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Role of the Localized Defect States in the Unconventional Magnetism of GaN and ZnO PRATIBHA DEV, PEIHONG ZHANG, Physics Department, University at Buffalo, Buffalo, NY 14260 — The cation defects -vacancies and the appropriate substitutionals - introduce localized defect states chiefly centered around the four surrounding anions in GaN and ZnO. This defect-induced magnetism in these otherwise nonmagnetic semiconductors is studied using ab-initio methods. The defects investigated include the cation vacancy, substitutional acceptors, and acceptor-like defect complexes. The defect states show two opposing attributes -one one hand, they are strongly localized on the anions surrounding the defect site, leading to local magnetic moment formation, while on the other hand, the extended tails of their wavefunctions lead to the long-ranged exchange interaction between the local moments.

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