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Defect-induced intrinsic magnetism in wide-gap III-nitrides¹ PEI-HONG ZHANG, PRATIBHA DEV, YU XUE, University at Buffalo, SUNY — Cation vacancy induced intrinsic magnetism in GaN and BN is investigated by employing density functional theory based electronic structure methods. The strong localization of defect states favors spontaneous spin polarization and local moment formation. A neutral cation vacancy in GaN or BN leads to the formation of a net moment of 3 μ_B with a spin-polarization energy of about 0.5 eV at the low density limit. The extended tails of defect wavefunctions, on the other hand, mediate surprisingly long-range magnetic interactions between the defect-induced moments. This duality of defect states suggests the existence of defect induced or mediated collective magnetism in these otherwise nonmagnetic sp systems.

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