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Electronic structure of Gd-doped GaN: vacancy-stabilized ferromagnetism PAUL LARSON, University of Missouri - Department of Physics & Astronomy, SASHI SATPATHY, University of Missouri - Department of Physics — The study of dilute-doped magnetic semiconductors has attracted significant interest recently, especially that of Gd-doped GaN. While experimental evidence for a colossal moment/Gd have been found in the low doping regime, we will focus on the stabilization of ferromagnetism over antiferromagnetism with much better understood 7–8 μ_B/Gd. Electronic structure calculations have been performed using the LAPW method within the WIEN2k code. Supercell calculations have shown that, in the absence of Ga or N vacancies, the large distance between Gd atoms leads to antiferromagnetism by the superexchange mechanism. Ga and N defects allows for extra electrons or holes to mediate the magnetism between the Gd atoms and stabilizes the ferromagnetic state. The degree of vacancies necessary to stabilize ferromagnetism has been approximated within a percolation model. This work is supported by the Air Force Office of Scientific Research.

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