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**Defect compensation determined magnetism in wide gap dilute magnetic semiconductors (DMS)** LIN-HUI YE, A.J. FREEMAN, DEPARTMENT OF PHYSICS & ASTRONOMY, NORTHWESTERN UNIVERSITY TEAM — Ferromagnetism (FM) in wide gap DMS is thought to be closely related to intrinsic defects; the F-center Bound Magnetic Polaron (FC/BMP) model proposes that it is mediated by shallow donor defects. Our first principles FLAPW calculations show that Cr:$TiO_2$ is a charge transfer insulator with strong defect compensation - which explains the insulating behavior and the Cr chemical valence. We predict different magnetic phases can form at different compensation levels, consistent with the $p-d$ hopping interaction model[1]. FM only exists with uncompensated $Cr^{4+}$, which explains the high $T_c$ FM initially reported[2]. Fully-compensated $Cr^{3+}$ is predicted NOT to be FM which has been verified recently[3]. Due to insufficient hybridization between dopant and impurity states, the FC/BMP mechanism does not apply, and oxygen vacancies destroy the FM instead of mediating it. Our theory extended to Mn:GaN is found to work equally well; it provides a new understanding of the correlation between defects and magnetism. This may explain why magnetism in wide gap DMS seems to be extremely sensitive to fabrication processes. Supported by NSF through the NU MRC.

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[2]T.Droubay *et al.* J.Appl.Phys. **97**, 046103 (2005)
[3]T.C.Kaspar *et al.*, Phys.Rev.Lett. **95**, 217203 (2005)

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