

Abstract Submitted
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Effect of vacancies on ferromagnetism in GaN:Mn dilute magnetic semiconductors from first principles¹ PAUL LARSON, SASHI SATPATHY, University of Missouri — In spite of considerable interest in ferromagnetism of the dilute magnetic semiconductor GaN:Mn, the nature of ferromagnetism is still quite controversial. Experimental values for the Curie temperature T_C vary widely depending upon the details of the the impurity concentrations. We have performed *ab initio* density functional studies of the magnetic interactions in GaN in the presence of nitrogen and gallium vacancies. Previous studies have found the nitrogen vacancy has the lowest formation energy. The nitrogen vacancy releases electrons in the system which changes the Mn d^4 state to a half-filled Mn d^5 state, so that the antiferromagnetic superexchange becomes dominant. The naive picture of Ga vacancies is the release of holes into the system which should increase ferromagnetism. However, we find an antiferromagnetic interaction for the Ga vacancy as well, in agreement with Mahadevan's work². This can be attributed to the localized nature of the hole states which do not participate in the transport. This hole localization from the Ga vacancy has been demonstrated using the virtual crystal approximation. Thus, both the nitrogen and gallium vacancy are found to impede ferromagnetism. This work is supported by AFOSR-FA 9550-05-1-0462.

¹P.Larson and S. Satpathy, submitted to Phys. Rev. B ²P. Mahadevan and S. Mahalakshmi, Phys. Rev. B **73**, 153201 (2006).

Paul Larson
University of Missouri

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