Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

The Failure of LDA and GGA to describe Relative Stability, Electronic Structure and Magnetism of MnN and (Ga,Mn)N Alloys[1]

JENNIFER CHAN, ZHE LIU, HANNES RAEBIGER, STEPHAN LANY, ALEX ZUNGER, NREL, Golden, CO 80401 — Pure MnN and (Ga,Mn)N alloys are studied using *ab initio* generalised gradient approximation $+U$ (GGA+U) or hybrid-exchange density functional (B3LYP) methods which predict dramatically different electronic structure, magnetic behavior and relative stabilities compared to local-density calculations. A unique structural anomaly of MnN, in which local-density calculations fail to predict the experimentally observed rocksalt as the ground state, is resolved with GGA+U and B3LYP. The phase-separation of zinc-blende (Ga,Mn)N alloys is examined using a mixed-basis cluster expansion based on the corrected GGA total energies. The predicted asymmetric spinodal phase diagram indicates that (Ga,Mn)N precipitates contain ∼5% or ∼50% Mn at typical growth temperatures. Thus, 100% pure MnN, that suppresses the Curie temperature, will not be formed. The Curie temperature for the x_{Mn}=50% phase is estimated to be T_C=∼300 K indicating that high T_C ferromagnetism in zinc-blende (Ga,Mn)N alloys is due to precipitates.
Chan *et al.* Phys. Rev. B **78**, 184109 (2008).

[1]Funded by the DOE-SC-BES-MSED and the DARPA-PROM program under NREL contract DE-AC36-08GO28308

Jennifer Chan
NREL, Golden, CO

Date submitted: 16 Dec 2008 Electronic form version 1.4