Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Magnetism and Doping in $GeMnN_2$ M. WEINERT, S. H. CHEUNG, L. LI, U. Wisconsin-Milwaukee — Although Mn doping has played a prominent role in the search for magnetic semiconductors, the development of new materials often has been hampered by phase segregation. To avoid this problem, compounds with high Mn concentrations are appealing, with $GeMnN_2$ being a promising candidate. We present Full-potential Linearized Augmented Plane Wave (FLAPW) calculations of the structural, electronic, and magnetic properties for both wurtzite and zincblende modifications. The ground state is found to be a semiconducting antiferromagnetically ordered "hexagonal" oP16 structure, with large local moments of $\sim$5 μ_B/Mn. The Mn atoms on the different magnetic sublattices are almost fully spin-polarized. Doping and/or intrinsic defects on the Mn sites effectively remove moments from the AFM background, resulting in a net *ferri*magnetic moment of 5 μ_B/Ge antisite; for Cu dopants, there is a net moment of 4 μ_B/Cu and the system becomes a half-metallic p-doped material.

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Date submitted: 01 Dec 2004 Electronic form version 1.4