Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Electronic structure of CrN: a Mott insulator ADITI HERWADKAR, WALTER R.L. LAMBRECHT, Case Western Reserve, MARK VAN SCHILFGAARDE, Arizona State University — It was recently reported by D. Gall et al. [J. Appl. Phys. 91, 5882, 2002] that CrN in the rocksalt structure has an optical band gap of about 0.7 eV, though in local spin density approximation, this materials is predicted to be metallic. We examine this possibility using the LSDA+U approach in the fully localized limit implemented in our full-potential muffin-tin orbital method. Slater integral $F^0 = U$ is screened such that the position of the occupied $3d$ levels agrees well with the photoelectron spectra of CrN. We find that a band gap opens in the band structure. The actual value of the gap obviously depends on the choice of U. To understand the origin of the gap it is essential to study how the d states split in cubic symmetry and what their filling is. Cr in forming CrN is trivalent and hence has three $3d$ electrons. The Cr e_g, form antibonding states in the conduction band. Adding U tends to push these empty states further up for both spins. The t_{2g} on the other hand form weaker π bonds with N $2p$, which in LSDA occur near the Fermi energy. Adding a Hubbard U now shift the majority spin electrons by $-U/2$ and the minority spin ones by $U/2$ and remove them from the Fermi level. This works because the three fold degenerate majority spin state $t_{2g\uparrow}$ becomes completely filled while the minority $t_{2g\downarrow}$ becomes empty. The valence band maximum then has predominantly N$2p$ character, which makes CrN a charge transfer type Mott-insulator.

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Date submitted: 02 Dec 2005 Electronic form version 1.4