Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Conducting states caused by a surface electric dipole in CrN(001) very thin films ANTIA S. BOTANA, VICTOR PARDO, DANIEL BALDOMIR, Departamento de Física Aplicada, Universidade de Santiago de Compostela, E-15782 Campus Vida s/n, Santiago de Compostela, Spain, PETER BLAHA, Institute of Materials Chemistry, Vienna University of Technology, Getreidemarkt 9/165-TC, A-1060 Vienna, Austria — The changes in the electronic structure of oxides and other correlated compounds caused by electronic reconstructions at their surface and interfaces has attracted much attention recently. CrN shows a magnetostructural phase transition as a function of temperature and controversial electronic properties. It has been argued recently that, with the onset of antiferromagnetic order, CrN as a bulk is always semiconducting, but very close to a metal-insulator transition [1]. In order to check if a small perturbation in the system could drastically change its conduction properties, we have performed electronic structure calculations for CrN in a thin film geometry within the LDA+U method. For thin films with increasing thickness (4-10 layers) starting with a critical thickness of 10 (cubic symmetry) or 6 layers (orthorhombic) the gap closes and conducting states appear. The appearence of metallic states is connected with a structural relaxation at the surface, where Cr (N) atoms buckle inside (outside) forming an effective surface dipole moment. Being CrN a low-gap system, these electric dipoles at the surface are able to shift the bands around the Fermi level significantly enough to drive those thin films metallic.

[1] A. S. Botana et al. Phys. Rev. B 85, 235118 (2012)

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Date submitted: 04 Dec 2012 Electronic form version 1.4