Electronic structure of CrN: from macro to nano.

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. In the bulk, calculations show that with the onset of magnetism, CrN is semiconducting but being 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 [2]. For free standing thin films with increasing thickness the gap closes and conducting states appear. The appearance 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. CrN being 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. From a theory standpoint, the study of CrN/MgO multilayers is the best scenario to study the effect of a drastic dimensionality reduction and the evolution of the electronic structure with thickness without conducting surface effects appearing that complicate the picture and prevent the study of quantum confinement effects alone. In contrast to the free CrN surface, CrN grown on MgO retains the semiconducting behavior shown in the bulk and even widens its band gap as the CrN thickness is reduced. Otherwise, interfacial effects with the oxide lead in this case to negligible electronic reconstructions with d-levels of the interfacial Cr atoms lower in energy due to the different environment present at the interface.

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

[2] A.S. Botana et al. Phys. Rev. B **87,** 075114 (2013)