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Electronic structure of CrN/MgO multilayers ANTIA S. BOTANA, University of California Davis, VICTOR PARDO, DANIEL BALDOMIR, Universidade de Santiago de Compostela, PETER BLAHA, Vienna University of Technology — 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. For free standing thin films with increasing thickness the gap closes and conducting states appear connected with a structural relaxation at the surface, where an electric dipole is formed. We report a series of electronic structure calculations for CrN/MgO multilayers within the LDA+U method. 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 to negligible electronic reconstructions. The d-levels of the interfacial Cr atoms are lowered in energy due to the different environment present at the interface. The evolution of the transport properties is analyzed and a significant enhancement of the Seebeck coefficient is predicted for the case of very thin CrN layers.

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