

Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Electronic and Magnetic Structure of CrO₂ and CrO₂-RuO₂ Interfaces¹ W. H. BUTLER, MINT Center, University of Alabama, HUNTER SIMS, Department of Physics, Tulane University, KRISHNA CHETRY, ZHIHONG LU, SANJOY SARKER, MINT Center, University of Alabama — CrO₂ and RuO₂ share the same (rutile) crystal structure and have similar lattice constants. We have used Density Functional Theory within both the generalized gradient and LDA+U approximations to calculate the electronic and magnetic structure of CrO₂, RuO₂ and their interfaces. Consistent with previous calculations and experiment we find (for both GGA and LDA+U) that the CrO₂ Fermi energy lies in a band gap for the minority channel. RuO₂, in agreement with experiment, is predicted to be a metal by both types of calculations. We find relatively good matching between the majority energy bands of CrO₂ and either channel of RuO₂ in the (100), (110) and (001) directions. The nearest neighbor exchange interaction in CrO₂ is calculated and used to estimate a Curie temperature of 411K. For (100) interfaces of CrO₂ and RuO₂, we find that the CrO₂ moments remain collinear if the interfaces are abrupt, but our models of intermixed interfaces yielded non-collinear moment configurations with neighboring Cr moments making an angle of approximately 150° and a small induced Ru moment oriented opposite to that of the sum of the Cr moments. We speculate that non-collinear spins at interfaces may be a common problem in oxides that may be a challenge to overcome to achieve large GMR and TMR effects in some of these materials.

¹Work supported by NSF MRSEC DMR0213985.

William H. Butler
MINT Center, University of Alabama

Date submitted: 30 Nov 2005

Electronic form version 1.4