Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

First principles study of the origin of Strain-tunable extraordinary magnetocrystalline anisotropy in Sr_2CrReO_6 epitaxial films M.R. BALL, The Ohio State University, J.M. LUCY, O.D. RESTREPO, OSU, A.J. HAUSER, UC, Santa Barbara, J.R. SOLIZ, OSU, J.W. FREELAND, Argonne National Lab, P.M. WOODWARD, W. WINDL, F. Y. YANG, OSU — Magnetocrystalline anisotropy (MCA) has significant implications in a range of applications such as power generation and magnetic data storage. We report the discovery of extraordinarily large anisotropy fields and strain-tunable MCA in Sr_2CrReO_6 epitaxial films. These films grown on $(LaAlO_3)_{0.3}(Sr_2AlTaO_6)_{0.7}$ (LSAT), $SrTiO_3$, and $SrCr_{0.5}Nb_{0.5}O_3$/LSAT substrates undergo dramatic changes in MCA shown by a shift in easy axis from in-plane to out-of plane. To find the origin of this, we determine the strain-induced distortions and octahedral rotations by performing density functional theory (DFT) calculations using VASP. Correlation effects were treated within GGA+U. In DFT, the change in easy axis under strain seen in experiment can be examined through the difference in total energies for magnetic orientation along different crystalline axes known as the magnetic anisotropy energy (MAE). The MAE is directly related to the moment anisotropy which is the difference between hard- and easy-axis orbital moments. When a sign change in the moment anisotropy is present, a change in easy axis is indicated. We indeed find this sign change with increasing c/a ratio which is in agreement with experiments. The origin of the MAE resides in the strain-induced changes in spin-orbit coupling on the Re-atoms. This interplay between structural deformations and magnetism leads to a giant MCA

Oscar Restrepo
The Ohio State University

Date submitted: 14 Nov 2014 Electronic form version 1.4