Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Crystal field splitting and optical band gap of hexagonal $LuFeO_3$ films[1] XIAOSHAN XU, Oak Ridge National Lab, WENBIN WANG, University of Tennessee, Oak Ridge National Lab, HONGWEI WANG, Temple University, University of Science and Technology of China, XIAOYING XU, Oak Ridge National Lab, LEYI ZHU, Argonne National Lab, LIXIN HE, University of Science and Technology of China, ELIZABETH WILLS, XUEMEI CHENG, Bryn Mawr College, DAVID KEAVNEY, Argonne National Lab, JIAN SHEN, Fudan University, University of Tennessee, XIFAN WU, Temple University — In order to study the electronic structures, we have characterized the hexagonal $LuFeO_3$ films (grown by pulsed laser deposition) using x-ray absorption and optical spectroscopy. The crystal splitting of Fe^{3+} is extracted as $E_{e'} - E_{e''}$=0.7 eV and $E_{a_1'} - E_{e'}$=0.9 eV and a 2.0 eV optical band gap is determined assuming a direct gap. First-principles calculations confirm the experiments that the relative energies of crystal field splitting states do follow $E_{a_1'} > E_{e'} > E_{e''}$ with slightly underestimated values and a band gap of 1.35 eV.

[1]Research supported by US DOE, Office of Basic Energy Sciences, Materials Science and Engineering Division

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Date submitted: 07 Nov 2012 Electronic form version 1.4