Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

First Principles Prediction of Topological Phases in Thin Films of Pyrochlore Iridates[1] XIANG HU, The University of Texas at Austin, ZHICHENG ZHONG, Vienna University of Technology, MEHDI KARGARIAN, The Ohio State University, ANDREAS RÜEGG, Theoretische Physik, ETH Zürich, PENGHAO XIAO, The University of Texas at Austin, CHANDRIMA MITRA, Oak Ridge National Laboratory, GREGORY A. FIETE, The University of Texas at Austin
— Using density functional theory and Hartree-Fock theory, we predict topological phases in thin pyrochlore iridate films grown along the [111] direction. Including the full orbital structure of the the relevant d-orbitals and the strong but finite-spin orbit coupling strength, we find a two-dimensional time-reversal invariant topological insulator with a gap of up to .15eV is possible in a bilayer geometry, and a zero magnetic field quantum anomalous Hall state is possible in a trilayer geometry with a gap of up to 0.1eV. Our results show that while the bulk pyrochlore iridates experimentally explored so far may not be promising for insulating topological phases, the thin film geometries are.

[1]The work is supported by ARO Grants No. W911NF-09-1-0527 and W911NF-12-1-0573, NSF Grant No. DMR-0955778 and DARPA grant D13AP00052.

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Date submitted: 13 Nov 2013 Electronic form version 1.4