Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Metal-Insulator Transition and Topological Phases of Pyrochlore Iridates RU CHEN, EUN-GOOK MOON, University of California, Santa Barbara , LEON BALENTS, Kavli Institute for Theoretical Physics, Santa Barbara — The 4d and 5d transition metal oxides are interesting because these materials incorporate both strong spin-orbit coupling and strong correlations, and consequently display distinct physical properties and the tantalizing possibility of novel topological phases. A prominent family in this class, the rare earth pyrochlore iridates, shows a metal-insulator transition and non-collinear complex magnetic ordering in the insulating state. We carry out magnetic band structure calculations using the GGA+U method, which reproduce the systematic trend that stronger order and larger gaps occur with decreasing rare earth radius. A corresponding paramagnetic band calculation shows that $Pr_2Ir_2O_7$ is a strong candidate for a nodal quadratic band touching state, in which the doubly degenerate conduction and valence bands touch at the zone center, right at the Fermi level. This suggests that $Pr_2Ir_2O_7$ is very sensitive to perturbations, such as time reversal symmetry or cubic symmetry breaking terms, giving rise to the possibility of many novel phases. Indeed, we demonstrate using first-principles calculations that uniaxial strain applied along the (111) direction opens a band gap and converts the material to a strong topological insulator.

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Date submitted: 15 Nov 2013

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