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First Principles Prediction of Topological Phases in Thin Films of
Pyrochlore Iridates

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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 relevant d-orbitals and the strong but finite-spin
orbit coupling strength, we find a two-dimensional time-reversal invariant topologi-
cal 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 ex-
perimentally explored so far may not be promising for insulating topological phases,
the thin film geometries are.

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