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Two-Dimensional Oxide Topological Insulator With LiFeAs Structure QIUNAN XU, ZHIDA SONG, SIMIN NIE, HONGMING WENG, ZHONG FANG, XI DAI, Chinese Academy of Sci (CAS), KEY LABORATORY OF CONDENSED MATTER THEORY AND COMPUTATION, CHINESE ACADEMY OF SCI, T03 GROUP TEAM — Using first-principles calculations, we propose that ZrSiO can be viewed as a three-dimensional (3D) oxide weak topological insulator (TI) with Z_2 invariants $(0; 001)$. Further calculations show that the single layer of such material is a long-sought-after 2D oxide TI with a band gap around 10 meV. Furthermore, we also find that there are many other isostructural compounds, which can host similar electronic structure and form a ‘WHM’ material family with ‘W’ being Zr, Hf or La, ‘H’ being group IV or group V element, and ‘M’ being group VI one.

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