Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Structurally unstable III-Bi-O_3 perovskites are predicted to be topological insulators but their stable structural forms are just band insulators: A first principles study[1] GIANCARLO TRIMARCHI, ARTHUR J. FREEMAN, Northwestern U., Evanston, IL, XIUWEN ZHANG, ALEX ZUNGER, U. of Colorado, Boulder, CO — Several Bi oxides in the assumed cubic $Pm\bar{3}m$ perovskite structure have recently been identified as topological insulators or semimetals by first-principles calculations. In these perovskites, Bi is at the octahedral site and the A atom at the interstitial site is a column III cation, i.e., Al, Ga, In, Sc, Y, La. We use density functional total-energy calculations and crystal structure prediction to determine the energetically stable phases for these oxides. We find that these $Pm\bar{3}m$ ABiO_3 perovskites are topological insulators, confirming recent results obtained by our and other groups. However, switching the position of Bi and A in the $Pm\bar{3}m$ perovskite produces trivial insulators or semimetals, as opposed to topological insulators. Indeed, symmetry-lowering via concerted tilting and internal deformation of the octahedra, stabilizes these Bi oxides, irrespective of the position of Bi, producing the stable $Pnma$ perovskite structure that is not a topological insulator. This illustrates that a simultaneous application of "first-principles thermodynamics" with first-principles electronic structure (Z_2 evaluation) is needed to establish stable topological insulators.

[1]Work at Northwestern supported by the DOE ER46536 grant; work at U. of Colorado, Boulder supported by the NSF DMR-1334170 grant.

Giancarlo Trimarchi
Northwestern University, Evanston, IL 60208

Date submitted: 15 Nov 2013 Electronic form version 1.4