Structurally unstable III-Bi-O\textsubscript{3} perovskites are predicted to be topological insulators but their stable structural forms are just band insulators: A first principles study\textsuperscript{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 \textit{Pm\textsubscript{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 \textit{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 \textit{Pm\textsubscript{3}m} \textit{ABiO\textsubscript{3}} perovskites are topological insulators, confirming recent results obtained by our and other groups. However, switching the position of Bi and \textit{A} in the \textit{Pm\textsubscript{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 \textit{Pnma} perovskite structure that is not a topological insulator. This illustrates that a simultaneous application of “first-principles thermodynamics” with first-principles electronic structure (\textit{Z\textsubscript{2}} evaluation) is needed to establish stable topological insulators.

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