Topological electronic structure in half-Heusler topological insulators\textsuperscript{1} WAEL AL-SAWAI, HSIN LIN, ROBERT MARKIEWICZ, Northeastern University, L. WRAY, Y. XIA, S. XU, M. HASAN, Princeton University, A. BANSIL, Northeastern University — We investigate the details of electronic band structure of a series of 28 ternary half-Heusler compounds MM'X of MgAgAs-type where M = (Lu, La, Sc, Y) and M'X=(PtBi, AuPb, PdBi, PtSb, AuSn, NiBi, PdSb). Our results show that the $\mathbb{Z}_2$ topological order is due to a single band inversion at the $\Gamma$-point. Half-Heusler compounds can be either topologically nontrivial semimetals, nontrivial metals, or trivial insulators. Our analysis reveals a straightforward relationship between the band inversion strength (extent of deviation from the critical point), the atomic charge of constituents, and the lattice parameter. Our findings suggest a general method for identifying $\mathbb{Z}_2$ topological insulators in nonmagnetic ternary compounds.

\textsuperscript{1}Work supported by the US DOE.