Abstract Submitted
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Toplogical electronic structure in half-Heusler topological insulators[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 Z_2 topological order is due to a single band inversion at the Γ-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 Z_2 topological insulators in nonmagnetic ternary compounds.

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