

Abstract Submitted  
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**Three Dimensional Topological Insulators on the Half-Heusler Lattice**<sup>1</sup> DI XIAO, Oak Ridge National Lab, XINGQIU CHEN, Oak Ridge National Lab & Institute of Metal Research, Chinese Academy of Science, WENGUANG ZHU, University of Tennessee & Oak Ridge National Lab, G. MALCOLM STOCKS, Oak Ridge National Lab, ZHENYU ZHANG, Oak Ridge National Lab & University of Tennessee — Using both tight-binding model and first-principles density functional theory, it is shown that a class of materials in the half-Heusler structure are topological insulators. Specifically, the  $Z_2$  topological index is evaluated based on the bulk magnetoelectric polarizability calculation and the surface-band structure is also obtained explicitly. We find there is a metal to topological insulator phase transition upon the application of pressure.

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