Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Half-Heusler Topological Insulators: A First-Principle Study with the Tran-Blaha Modified Becke-Johnson Density Functional[1] WANXIANG FENG, Institute of Physics, Chinese Academy of Sciences, DI XIAO, Oak Ridge National Lab, YING ZHANG, Beijing Normal University, China & University of Texas, YUGUI YAO, Institute of Physics, Chinese Academy of Sciences & University of Texas — We systematically investigate the topological band structures of half-Heusler compounds using first-principles calculations. The modified Becke-Johnson exchange potential together with local density approximation for the correlation potential (MBJLDA) has been used here to obtain accurate band inversion strength and band order. Our results show that a large number of half-Heusler compounds are candidates for three-dimensional topological insulators. The difference between band structures obtained using the local density approximation (LDA) and MBJLDA potential is also discussed.

[1]Research sponsored by the Department of Energy, Office of Basic Energy Sciences, Materials Sciences and Engineering Division, and Institute of Physics, Chinese Academic Science

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Date submitted: 17 Nov 2010 Electronic form version 1.4