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Stable nontrivial Z_2 topology in ultrathin Bi (111) films: a first-principles study[1] ZHENG LIU, Tsinghua University & University of Utah, CHAO-XING LIU, Wuerzburg Universitat, YONG-SHI WU, University of Utah, WEN-HUI DUAN, Tsinghua University, FENG LIU, University of Utah, JIAN WU, Tsinghua University — Recently, there have been intense efforts in searching for new topological insulator (TI) materials. Based on first-principles calculations, we find that all the ultrathin Bi (111) films are characterized by a nontrivial Z_2 number independent of the film thickness, without the odd-even oscillation of topological triviality as commonly perceived. The stable nontrivial Z_2 topology is retained by the concurrent band gap inversions at multiple time-reversal-invariant k-points and associated with the intermediate inter-bilayer coupling of the multi-bilayer Bi film. Our calculations further indicate that the presence of metallic surface states in thick Bi(111) films can be effectively removed by surface adsorption.

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