Topological surface states of the Heusler topological insulators

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Many Heusler compounds were theoretically predicted to be topological insulators (TIs) with multi-functionalities such as the noncentrosymmetric superconductivity. However, the existence of their topological surface states still remains elusive. We have performed systematical ab initio band structure calculations for Heusler TI compounds YPtBi, LaPtBi and LuPtB and successfully revealed their topological surface states. Different from a common TI where the topological states exist near the Fermi energy, Heusler topological surface states appear inside the deep valence bands due to the lack of a bulk energy gap. Trivial surface states exist across the Fermi energy with giant Rashba spin split, which can be attributed to surface dangling bonds. Our work explains why previous ARPES failed to detect the topological surface states at the Fermi energy and present a guidance for future experiments to address the topological states unambiguously.