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Topological Phase Transition in Antimony[1] MAN-HONG WONG, GUANG BIAN, CAIZHI XU, THOMAS MILLER, TAI-CHANG CHIANG, University of Illinois at Urbana-Champaign — Spin-orbit coupling (SOC) is believed to cause the parity exchange that drives normal band insulators into the topological regime. Changing the strength of the effective SOC can also induce quantum phase transitions in materials. We performed a first-principles calculation to elucidate the quantum phase transition from a topologically trivial to nontrivial system in a 15-bilayer Sb film. We increased the k-space sampling relative to previous studies and varied the effective SOC in order to observe the changes in the bulk band gap and topological surface states. A transition from a metal to a semimetal is observed as the SOC is tuned from 0% to 100%. At a SOC value near 300%, a transition from a nontrivial topological semimetal to a topological insulator occurs. Varying the effective SOC strength can be realized experimentally by alloy substitution with elements in the same column in the periodic table. Increasing the effective SOC of the Sb film to values above 100% is a model of the $Bi_{1-x}Sb_x$ alloy, the first three-dimensional topological insulator. Further studies using this method on different systems may lead to the discovery of new topological insulators.

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