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Topological insulator with negative spin-orbit coupling XIAN-LEI SHENG, Univ of Delaware, ZHIJUN WANG, RUI YU , HONGMING WENG, ZHONG FANG, XI DAI, Institute of Physics, Chinese Academy of Sciences, KEY LABORATORY OF CONDENSED MATTER THEORY AND COMPUTATION TEAM — Based on the first-principles calculations, we reveal that TlN, a simple binary compound with Wurtzite structure, is a three-dimensional (3D) topological insulator (TI) with effectively negative spin-orbit coupling $\lambda_{eff} < 0$, which makes it distinguished from other TIs by showing opposite spin-momentum locking effect in its surface states. The sign of λ_{eff} depends on the hybridization between N-2p and Tl-5d states, and can be tuned from negative to positive by lattice strain or chemical substitution, which drive the system into a Dirac semimetal with 3D Dirac cones in its bulk states. Such topological phase transition can be realized by electronic mechanism without breaking any crystal symmetry.

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