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Topological phases in rocksalt rare-earth binary compounds¹ HSIN LIN, MINGGANG ZENG, GUOQING CHANG, National University of Singapore, YU-AN CHEN, TIMOTHY HSIEH, Massachusetts Institute of Technology, ARUN BANSIL, Northeastern University, LIANG FU, Massachusetts Institute of Technology — Using first-principles calculations, we have investigated the electronic properties of bulk lanthanum monopnictides (LaX, X = N, P, As, Sb, Bi) and their thin films. We predict that lanthanum nitride (LaN) harbors a three-dimensional (3D) Dirac semimetal phase, and undergoes a phase transition driven by Coulomb interaction. Other lanthanum monopnictides are found to be semimetals with a non-trivial Z2 band topology. Furthermore, we find both two-dimensional (2D) Dirac semimetal and topological insulator phases in thin films of lanthanum monopnictides. The gapless Dirac states in bulk lanthanum monopnictides and their thin films can be attributed to the crystalline symmetry protection.

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