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First-principles study of atomic structures and electronic properties of Bi ultrathin films on Ge(111) CHIA-HSIU HSU, HUA-RONG CHANG, FENG-CHUAN CHUANG, YU-TZU LIU, ZHI-QUAN HUANG, Department of Physics, National Sun Yat-Sen University, Kaohsiung 804, Taiwan, HSIN LIN, Graphene Research Centre and Department of Physics, National University of Singapore, Singapore 117542, VIDVUDS OZOLINS, Department of Materials Science and Engineering, University of California, Los Angeles, Los Angeles, California 90095-1595, USA, ARUN BANSIL, Department of Physics, Northeastern University, Boston, Massachusetts 02115, USA — The atomic and electronic structures of ultrathin bismuth films on Ge(111) surface were investigated using first-principles calculations at Bi coverages ranging from 1/3 ML to 5 ML. Morphology of the surfaces varied as the coverage of Bi was increased. We found that the first layer of bismuth atoms follows the well-known trimer model exhibiting large Rashba spin-splittings. At 2 ML, bismuth atoms of the second monolayer form the second stacking layer of trimers, whereas at 3 ML and 5 ML, bismuth atoms of the topmost two monolayers form a buckled honeycomb structure. While the electronic structures of the two topmost layers exhibit two-dimensional nontrivial topological insulating phase, the bismuth atoms lying under these layers play an important role in p-type doping of the system.

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