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Direct imaging of band profile in single layer MoS2 on graphite: metallic edge states and the lateral Schottky barrier CHENDONG ZHANG, Department of Physics, the University of Texas, Austin, TX 78712, CHANG-LUNG HSU, YONG-HUANG CHANG, LAIN-JONG LI, Institute of Atomic and Molecular Sciences, Academia Sinica, Taipei, 10617, Taiwan, CHIH-KANG SHIH, Department of Physics, the University of Texas, Austin, TX 78712 — Recently, single layer (SL) Transition metal dichalcogenides MX_2 has attracted intense interests as the band structures change from indirect to direct gap. In addition, the valley degeneracy is also lifted in SL MX_2. These properties have important implications in nanoelectronics and optoelectronics. The SL MX_2 islands often come with a triangular form with straight edges and it has been shown theoretically these are zig-zag edge with metallic states. Here we use scanning tunneling microscopy/spectroscopy (STM/S) to map out the electronic structure of single layer MoS_2 grown on HOPG (highly oriented pyrolytic graphite) using CVD. In the region away from the edge, the MoS_2 band profile shows a homogeneous band gap of about 1.95 ± 0.1 eV, consistent with the optical studies before. Moreover, the Fermi level locates at 0.15 ± 0.05 eV below the conduction band minimum (CBM), confirming its n-type nature. The band profile is bend upward by about 0.5 eV within 5 nm from the edge. At the edge, the metallic nature is observed from finite conductivity in the gap region. This study shows that the bulk SL MoS_2 and its metallic edge formed a lateral Schottky barrier with a narrow depletion region of 5 nm and the Fermi level is pinned at 0.65 eV below the CBM.

Chendong Zhang
Department of Physics, the University of Texas, Austin, TX 78712

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