Electron-state Tuning of MoS2 Thin Film by Electrostatic and Chemical Doping

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Abstract

Molybdenum disulfide (MoS2) has been attracted a lot of research interests because of its two-dimensional layer structure, intrinsic band-gap, and optical properties. Recent experiments observed the superconductivity in this insulator material at a transition temperature of 11 K, by using the electrostatic electron doping technique [1]. However, the mechanism of this superconductivity behavior is still unclear. Therefore, in this work, we investigate the electronic structure of MoS2 ultrathin film under electrostatic or chemical doping based on the first-principles total-energy calculations [2]. Under the electrostatic electron or chemical doping, we find that the unoccupied nearly-free-electron (NFE) states shift downward, and finally crosses the Fermi level due to the strong electric field induced by accumulated charge near the surface. Because of this shift to lower energy due to electrostatic or chemical doping, the NFE state acts as the conducting channel for the injected carrier. These results indicate that the free-electron-like carriers play crucial roles in determining the superconductivity properties of MoS2, as in the case of intercalated graphite materials.

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