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Nonmetal-metal transition in anatase Nb-doped TiO_2 TARO HITOSUGI, Advanced Institute for Materials Research, Tohoku University, HIDEYUKI KAMISAKA, KOICHI YAMASHITA, HIROYUKI NOGAWA, TETSUKAZU TSURUHAMA, Univ. of Tokyo, SHOICHIRO NAKAO, YUTAKA FURUBAYASHI, NAOOMI YAMADA, Kanagawa Academy of Science and Technology (KAST), YASUSHI HIROSE, TOSHIHIRO SHIMADA, TETSUYA HASEGAWA, Univ. of Tokyo — Anatase TiO_2 show nonmetal-metal transition on Nb doping. Epitaxial $Ti_{0.94}Nb_{0.06}O_2$ (TNO) thin film exhibits low electrical resistivity, $\rho \sim 1.7$ x 10^4 Ωcm at 300 K, comparable to highly-conducting transition metal oxide, ReO_3 and Na_xWO_3. This TNO is an n-type degenerate semiconductor with carrier density exceeding 10^{21} cm^{-3}. We have studied the electronic structure of this TNO system using resonant photoemission spectroscopy and compared with first-principles calculations. The first-principles calculations reveal that there is no impurity state arising from Nb doping, and partial density of states of Nb contribute to both valence band and conduction band. These results imply that Nb is highly-hybridized with Ti and O orbitals, resulting in high activation efficiency of Nb which leads to high carrier density in the TNO system. Resonant photoemission spectra clearly show wide band gap without impurity state with Fermi edge located in the conduction band.

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