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Theoretical Study of Tip-Induced Band Bending and Local Tunneling Barrier Height on H-Terminated Si(100) Surface HIDEOMI TOTSUKA, Nihon University, SATOSHI WATANABE, The University of Tokyo, CREST TEAM — In scanning tunneling microscopy (STM) measurements on semiconductor surfaces, tip-induced band bending (TIBB) occurs due to the applied high bias voltage, and influences the local electronic structures of the surface detected by STM and scanning tunneling spectroscopy (STS). Recently, Yoshida et al. have reported the effect of the TIBB on local tunneling barrier height (LBH) on Si(100) surfaces by light-modulated STS [1]. However, theoretical studies on the TIBB and LBH have not been performed yet on semiconductor surfaces. In this study, we have analyzed the TIBB and LBH on an H-terminated Si(100) surface theoretically using the boundary-matching scattering-state density functional method [2], which can calculate the electron states under applied bias voltages self-consistently. In particular, we focus on the bias voltage dependences of the TIBB and LBH, and show that measured LBHs can be basically understood as the sum of TIBB and intrinsic barrier height. [1] S. Yoshida, et al., e-J. Surf. Sci. Nanotech. 4, 192 (2006). [2] Y. Gohda et al., Phys. Rev. Lett. 85, 1750 (2000). [3] M. McEllisterm, et al., Phys. Rev. Lett. 70, 2471 (1993).

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