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First-principles study of local p(2×2) structures on Si(100) surface MIN-KOOK KIM, HYOUNG JOON CHOI, Department of Physics and IPAP, Yonsei University — We study structural defects inducing local p(2×2) structures in c(4×2)-reconstructed Si(100) surface, using an *ab-initio* pseudopotential density functional method. The local density approximation to the density functional theory is used and electronic wavefunctions are expanded with pseudo-atomic orbitals. The atomic structures of defects are optimized by minimizing the total energy. Our calculations show that the defects increase the total energy of the system but they are energetically stable with energy barrier. STM images for occupied and unoccupied states are simulated to investigate the surface electronic structures. Effects of electron doping and external electric field on the defects are also studied. This work was supported by the KRF (KRF-2007-314-C00075) and by the KOSEF Grant No. R01-2007-000- 20922-0. Computational resources have been provided by KISTI Supercomputing Center (KSC-2008-S02-0004).

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