Atomic and Electronic Structure of Si(100)-(2x1)

Myung-Ho Kang

Department of Physics, Pohang Institute of Science and Technology

The atomic structure of the Si(100)-(2x1) surface has long been a challenging subject of semiconductor surface physics, both experimentally and theoretically. However, the equilibrium dimer geometry of this surface is still in question. A recent STM study [1] demonstrated well the symmetric-dimer domain in a defect-free region of Si(100). On the other hand, however, a more recent low-temperature STM study [2] strongly suggests that the asymmetric dimer is the equilibrium configuration of Si(100) at zero temperature. In theory parts, while early-day calculations proposed the asymmetric dimer model mainly based on the surface electronic structure argument, most of recent total-energy calculations, since the STM study of Ref.[1], are in favor of the symmetric-dimer model based on the energetics consideration.

We reexamine here the energetics of the dimer reconstruction of Si(100) by carrying out a more rigorous pseudopotential planewave-basis density-functional total-energy calculations. To deal with a small energy difference between the symmetric and asymmetric dimer configurations accurately, we choose the quality parameters such as supercell size, planewave cutoff energy, and k-point sampling very carefully through convergence tests. We determine the equilibrium dimer geometry both in symmetric and in asymmetric configurations using the Hellman-Feynman force scheme. Our total-energy calculations show that the asymmetric dimer geometry is more stable than the symmetric one by about 0.2 eV/ dimer. The surface bonding geometry related to the dimer asymmetry will be given. We will also mention briefly the surface core-level shifts on Si(100), a controversial subject of recent XPS studies [3-5], in the context of pseudopotential scheme, based on the hartree-potential change at surface atom cores.

[1] R. M. Tromp, R. J. Hamers, and J. E. Demuth, Phys. Rev. Lett. 55, 1303 (1985).

[2] R. A. Wolkow, Phys. Rev. Lett. 68, 2636 (1992).

[3] D. S. Lin, T. Miller, and T. C. Chiang, Phys. Rev. Lett. 67, 2187 (1991).

[4] J. E. Rowe and G. K. Wertheim, Phys. Rev. Lett. 69, 550 (1992).

[5] E. Landmark, C. Karlsson, Y. Chao, and R. Uhrberg, Phys. Rev. Lett. 69, 1558 (1992).