[Ⅲ~2]

The atomic structure of the Sb-induced Si(111)-5√3 × 5√3 surface: *ab initio* calculations

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In a recent scanning tunneling microscopy (STM) study,[1] a $5\sqrt{3} \times 5\sqrt{3}$ phase was observed with Sb deposition on Si(111) surfaces. Based on the analysis of STM images, an atomic arrangement for the Sb-induced $5\sqrt{3} \times 5\sqrt{3}$ structure was suggested, which consists of three 5×5 base structures; a single-adatom unfaulted half, two three-adatom unfaulted halves, and three faulted halves. In this work, we employ an *ab initio* pseudopotential method to determine the atomic structure corresponding to the observed STM images. Optimized geometries for several possible atomic structures are obtained from total-energy calculations. Furthermore, simulated STM images, including their bias-voltage dependence, are compared with experimental observations. The chemical identity of the adatoms, which comprise the $5\sqrt{3} \times 5\sqrt{3}$ structure, is determined by comparing calculated STM images of both Si- and Sb- adatom structures with the experimentally observed ones. The origin of bias-voltage dependent STM images is also discussed.

[Reference]

1. K.-H. Park, J. S. Ha, W. S. Yun, E.-H. Lee, J.-Y. Yi, and S.-J. Park "Atomic structure and formation kinetics of the Sb/Si(111) - $5\sqrt{3} \times 5\sqrt{3}$ surface", Phys. Rev. B **55**, 9267 (1997).