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Honeycomb-Chain Reconstruction of the High-Index Si (5 5 12) Surface: A First-Principles Study

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Exploration of stable crystalline surfaces with respect to a surface orientation poses a fundamental issue associated with equilibrium crystal shape and crystal growth, which play important roles in pure and applied fields. It is well known that the stability of a semiconductor surface is sensitive to surface reconstruction and governed by a delicate balance between minimization of the number of dangling bonds and the relief of surface stress. For Si, well-established structure models exist for only a couple of stable orientations, (001), (111), (113), and (114), and a few competing models for (5 5 12) that is recently found by scanning-tunneling microscopy (STM). The Si(5 5 12) surface is novel in that it has an extraordinarily high-index, resulting in a huge lattice size of 53.5 Å, and forms a planar surface with stable reconstruction in contrast to usual high-index surfaces that transform into bunched steps or facets in equilibrium. Furthermore, due to its structural regularities of one-dimensional (1D) chains and its hierarchy for metal adsorption, the Si(5 5 12) surface has attracted very much attention as a template for fabricating 1D metal nanowires with linewidth of true single nanometer scale.

In this paper, we present pseudopotential total-energy calculations on the atomic structure for the Si(5 5 12)2×1 surface. We construct a structure model by a bond-breaking and rebonding mechanism, as found in formation of the π-bonded chains of Si(111)2×1, and then obtain its equilibrium structure that contains honeycomb chains, dimers, adatoms, and tetramers. The present model, with the lowest energy among all other structure models, shows perfect agreement with STM, high-resolution transmission electron microscopy, and photoemission studies.