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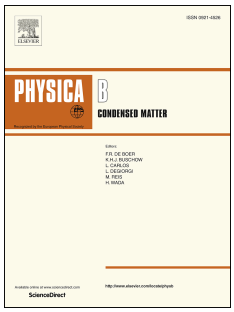

Co on the H-passivated Si(001) surface: Density-functional calculations

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Co on the H-passivated Si(001) surface: Density-functional calculations

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Abstract

We have presented an atomic and electronic structures, as well as chemical bonding of Co on the bare, partially H-passivated, and fully H-passivated Si(001)-(2×2) surface using density functional theory. There have been considered three different sites for Co on the surface; (1) an *l*-site (Co bonded to the lower lying Si-dimer component), (2) an *h*-site (Co bonded to the higher lying Si-dimer component), and (3) an *i*-site (intrarow position between adjacent Si dimer rows). The calculations indicate that for the *i*-site, the Co atom is located at nearly the same height as the Si dimers towards the vicinal region on the bare and partially H-passivated Si(001) surface. For all the remaining cases studied here, the Co atom prefers to stay at the subsurface site.

Keywords: Density Functional Theory, Adsorption, Silicon, Surface, Electronic Structure, Chemical potential

1. Introduction

A transition metal silicides, such as $CoSi_2$, play an important role in semiconductor industry due to its attractive properties such as low resistivity, thermal stability and good epitaxial alignment with a Si substrate [1, 2, 3, 4, 5, 7, 8, 9, 10, 11, 12, 13]. One of the experimental study by Scheuch *et al.* [1] investigated the first stages of $CoSi_2$ formation on the Si(001) surface. They provided detailed structural information from very low coverages of 0.01 monolayer (ML) to 30 ML coverage on Si(001). At higher coverage of Co, they found the formation of different two and three-dimensional islands. Pan *et al.* [2] studied Co deposition on both bare and hydrogen passivated Si(001)

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