

Adsorption Geometry of Na on Si(100)-(2x1)

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Recently, there has been strong attention on the atomic and electronic structure of the alkali-metal adsorbed Si(100) surfaces as a prototype of metal-semiconductor interfaces. However, since the results of many studies are conflicting one another, any conclusive information on the adsorption geometry and the nature of adsorbate-substrate interaction is not available at present. We report here the adsorption site and the corresponding bond length of Na on Si(100) investigated by carrying out the *ab initio* pseudopotential density-functional total-energy calculations.

We have studied the adsorption sites and bond lengths of Na (at half monolayer coverage) on a rigid (2x1) Si(100) substrate which was reconstructed within the standard symmetric-dimer reconstruction model. We find the quasihexagonal pedestal site is the most stable for adsorption and there the Na-Si bond length corresponds to 2.85Å. This bond length suggests following the atomic radii argument that at this coverage the nature of Na-Si interaction is not ionic, but weak covalent. Our result is in a good agreement with that of a recent LEED analysis, but disagrees to the previous pseudopotential calculations.

To study how the Na adsorbate modifies the clean-surface geometry, we fully relax the atomic positions of the adlayer and the top three substrate layers using the calculated Hellmann-Feynmann atomic forces. The effects of the substrate relaxation to the adsorption geometry will be discussed.

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