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First-principles study of the alkali-metal-adsorbed Si(111)3×1 surfaces

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This paper describes the application of the density-functional pseudopotential total-energy formalism to the alkali-metal (AM)- and alkaline-earth-metal (AEM)-adsorbed Si(111)3×1 surfaces.

The AM/Si(111)3×1 surfaces have been studied intensively because of their unique structural, electronic, and chemical properties. Although several structural models were suggested to explain the observed facts, none of them has been confirmed either theoretically or experimentally. We investigate the atomic and electronic structures of the AM (Na,K)/Si(111)3×1 surfaces within structural models proposed to date: the missing-top-layer (MTL), the overlayer, and the π-bonded chain models. Based on the energetics and the comparison of electronic structures between the calculation and experiment, we propose the MTL model as the ground-state structure of the AM/Si(111)3×1 surfaces. The buckled MTL structure is characterized by the linear chain of AM atoms adsorbed on a stable threefold-filled site between the buckled Si chains, and the large buckling induces a large surface-state band gap. We demonstrate that this model provides a consistent theoretical explanation of the measured properties.

We also study the Mg/Si(111)3×1 surface for structural models proposed for the AEM and AM cases. The total energy calculation shows that the overlayer and the MTL models with the threefold hollow adsorption site have the similar lowest energies, but the electronic structure comparison between the calculation and experiment prefers the overlayer model. The overlayer model has a half-filled surface-state band (*i.e.*, metallic), but its dispersion is so small that the Coulomb correlation may be important in this system. The large Hubbard correlation energy estimated by a charge transfer method is possibly the origin of the experimental semiconducting electronic structure.