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First-principles study of the atomic and electronic structure of the Si(111)-(5×2)-Au surface reconstruction

Chung-Yuan Ren,[1,*] Shiow-Fon Tsay,[2] and Feng-Chuan Chuang[2]
[1]*Department of Physics, National Kaohsiung Normal University, Kaohsiung, Taiwan 824*
[2]*Department of Physics, National Sun Yat-sen University, Kaohsiung, Taiwan 804*

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An alternative model for the Si(111)-Au reconstruction at 2/5 Au coverage is proposed and analyzed using first-principles calculations. This model is based on the structure suggested by Riikonen and Sánchez-Portal [Phys. Rev. B **71**, 235423 (2005)], but its periodicity of 5×2 is characterized by the removal of one silicon atom from every 5×2 supercell. It is found that this model and that of Erwin [Phys. Rev. Lett. **91**, 206101 (2003)] are very close energetically (<0.5 meV/Å^2). The key features of angle-resolved photoemission measurement and scanning tunneling microscopy are accounted for in this model. Particularly, the present model reproduces the surface band observed just below the Fermi level. Extra Si adatoms supply electrons that dope this weaker band and cause the system to convert from metallic to insulating, consistent with recent two-phase findings. The occupation of the silicon adatom on the parent surface is calculated to be at most one adatom per two 5×2 unit cells, in agreement with experiment.

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The electronic properties of low-dimensional systems are fundamentally different from those in higher dimensions due to unusually collective excitations.[1–4] In reality, the fabrication of metallic chains on surfaces leads to one- or two-dimensional characters of electronic states. One example is the vicinal Si(111)-Au surface, which provides options for tailoring the electronic states of gold chains by changing the miscut angle.[5–10] Even more widely studied is the parent flat Si(111)-Au. As a prototypical metal-semiconductor surface system, this structure shows a variety of reconstruction phases[11–14] and has attracted much attention in recent years.

Among the various reconstruction phases, the Si(111)-(5×2)-Au occurs at about 0.4 monolayer gold coverage.[15] Since first reported about three decades ago,[16–18] the Si(111)-(5×2)-Au surface reconstruction has been extensively investigated by low-energy electron diffraction,[16–18] x-ray diffraction,[19] scanning tunneling microscopy (STM),[20–28] angle-resolved photoemission spectroscopy (ARPES),[29–33] inverse photoemission,[34] core-level spectroscopy,[35] and high-resolution electron microscopy with heavy-atom holography.[36] Despite many studies, its atomic structure still remains under debate. The experimental results provide severe constraints on theoretical models for the Si(111)-(5×2)-Au surface.

Experimentally, STM studies show a series of Y-shaped features with correct crystallographic orientations[20–22] as well as the so-called bright protrusions (BPs).[23–28] BPs reside on the 5×2 structure with a preferred spacing of four lattice constants along the chains, rendering the local periodicity 5×4. However, they randomly occupy only half of the available lattice sites[25–28] (*a priori* properties required in a possible atomic scale memory[26]). Furthermore, photoemission reveals a strong surface band beginning at the 5×2 zone boundary and dispersing downward toward the 5×1 zone boundary.[30–33] The dispersion of this band is one dimensional[31–33] near the top of the band and gradually becomes two dimensional toward the bottom.[31] Weaker surface bands with one-dimensional character near the Fermi level (E_F) are also reported.[32,33] This observation makes it unclear whether the Si(111)-(5×2)-Au is metallic or semiconducting.[22,32,33]

Many earlier structural models were not compatible with detailed STM investigation[23] and the knowledge of more precise gold coverage.[15] Two later models, as suggested by Marks-Plass [36] (MP) and Haegawa-Hosaka-Hosoki (HHH),[24] have been examined theoretically.[37,38] However, neither was found to be consistent with the STM or ARPES data. Recently, Erwin[38] (E) and Riikonen–Sánchez-Portal[39] (RS) proposed two improved models, both of which show the honeycomb-chain (HC) feature,[38] yet with different alignments of the two Au rows. Besides having lower surface energies than those of the MP and HHH models, the band structure calculations of these two models seem to satisfy the main features of the empirical evidence. However, the observed weaker bands[32,33] close to E_F are either not attainable or their characteristics have not been investigated thoroughly.

In this work, we propose an alternative candidate model for the Si(111)-(5×2)-Au surface reconstruction.[40] As illustrated in Fig. 1, this model is based on the RS 5×1 model.[39] Instead of the appearance of the asymmetric rise of atoms in certain silicon rows in the original RS (5×2) variant, one silicon atom per 5×2 cell is removed in the present model to make periodicity 5×2. It is found that the present model is energetically very close to the Erwin model and explains the main features observed in the STM and ARPES data. It will be shown below that, when the surface is decorated by extra Si adatoms, the calculated metallic surface band near E_F is pushed down below E_F, making the full system insulating. This result is consistent with the recent findings of a series of alternating metallic and semiconducting segments along the chains.[22,33] The preferential Si-adatom content occurs for at most one adatom per two 5×2 cells. The surface energy differences among the cases of lower adatom densities are found to be rather minor, presumably reflecting the random

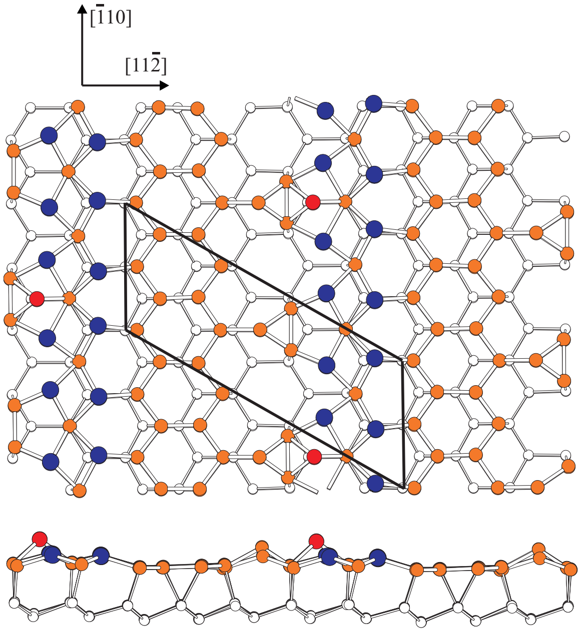

FIG. 1. (Color online) Atomic structure of the present model for the Si(111)-(5×2)-Au surface reconstruction. Blue, orange, and white circles represent gold, surface silicon, and underlying silicon atoms, respectively. The elementary 5×2 unit cell is outlined. Extra Si adatoms, represented by red circles, are also illustrated with 5×4 periodicity.

TABLE I. Surface energies (meV/Å^2) of the present model for Si(111)-Au surface reconstruction at 2/5 Au coverage. The results of the Erwin model (Ref. 38) are also listed for comparison. The energies presented here are relative to that of the Erwin 5×2 model with no adatoms.

	Adatom-free		One Si adatom		
Model	5×1	5×2	5×2	5×4	5×6
Present	−2.79	+1.14	+2.52	+0.65	+0.62
Erwin	+0.87	0.00	+0.52	+0.23	+0.21

distribution of the BPs on the Si(111)-(5×2)-Au surface.

First-principles total-energy calculations were carried out to investigate the atomic structures and relative surface energies of the models under consideration. The calculations were performed self-consistently in a slab geometry with three bilayers of Si plus the surface layer. Additional hydrogen atoms were chosen to saturate the dangling bonds of silicon atoms at the bottom of the slab. A vacuum region of ~12 Å ensured negligible interactions between neighboring slabs. Total energies and forces were determined within the generalized gradient approximation (GGA) to the density functional theory (DFT) using projector-augmented-wave potentials, as implemented in VASP code.[41,42] The plane-wave basis set with an energy cutoff of 312 eV was used. The 2×4, 2×3, and 2×2 Monkhorst-Pack grids were taken to sample the surface Brillouin zones (BZs) of the 5×2, 5×4, and 5×6 supercells, respectively. The Si atoms of the bottom bilayer were kept fixed at the bulk ideal positions, where the calculated lattice constant was set to be 5.466 Å. The remaining Si and Au atoms were relaxed until the total energy changed by less than 1 meV per 5×2 cell and the residual force was smaller than 0.02 eV/Å. To compare the stability of the present model with previous ones, we computed the surface energy, $E_s=(E_{t,5\times n}-N_{\mathrm{Au}}E_{\mathrm{Au}}-N_{\mathrm{Si}}E_{\mathrm{Si}})/A_{5\times n}$, where $E_{t,5\times n}$ is the total energy of a reconstructed 5×n supercell ($n=2,4,6$) containing N_{Au} Au and N_{Si} Si atoms, and E_{Au} and E_{Si} are the total energies per atom of bulk Au and Si, respectively. Here, $A_{5\times n}$ is the top surface area of a 5×n supercell. The spurious contribution of the hydrogen-terminated surface will not affect the relative surface energies since the Si atoms of the bottom bilayer and the hydrogen atoms were kept fixed during relaxation. The models and their variants considered here have equal Au coverage, hence the relative surface energies do not require a choice of Au chemical potential.

We first reexamined the Erwin model (Fig. 1 in Ref. 38). The band structure and STM image of the $E(5\times2)$ adatom-free model obtained by Erwin[38] were well reproduced in the present calculations. With inclusion of Si adatoms, the resultant most stable atomic structure is also similar to earlier work.[38] We then turned to study in detail the model proposed by Riikonen and Sánchez-Portal.[39] The basic RS model shows a clear HC feature, which appears in the Erwin model as well. However, the gold rows are arranged in a rather different way (Fig. 8 in Ref. 39). The separation between the two gold rows is 3.10 Å, smaller than the value of 3.80 Å found in the Erwin case. Table I shows that the surface energy of the RS (5×1) variant is lower than that of the $E(5\times1)$ by an appreciable amount of 3.66 meV/Å^2. In addition, we performed the band structure calculations of the RS (5×1) model along the gold chain. Figure 2(a) plots the results with wave vectors specified in the two-dimensional BZ [Fig. 2(b)]. Clearly, the most predominant surface band between the 5×2 and 5×1 boundaries is well reproduced (labeled S_1). As compared to previous experiments,[30–33] the bandwidth of this band is improved from the earlier result[38] of 0.6 eV to 1.1 eV and the location of the band is more correct. The less dispersive band S_3 is also easily identified in the experiment.[32] More importantly, the ARPES data reveal another weaker surface band near E_F,[32,33] which is closely related to the debate of whether the Si(111)-(5×2)-Au surface is metallic or semiconducting. Figure 2(a) shows just such a band, S_2. Combined with the energetic advantage mentioned above, the RS (5×1) atomic structure is appealing and instructive. This model seems to serve as another good starting point to construct potentially "correct" models to account for the detailed experiments of the complex Si(111)-(5×2)-Au surface.

As suggested by Riikonen and Sánchez-Portal,[39] the periodicity of the RS (5×2) is characterized by one of every two atoms in one silicon row of the HC structure appearing at a higher position with respect to the other (Fig. 8 in Ref. 39). However, if this is the case, from the atomic structural point of view, it seems difficult to stimulate *only one* clear Y-shaped feature in one 5×2 unit observed in the STM image. Moreover, the present calculations show that the origi-

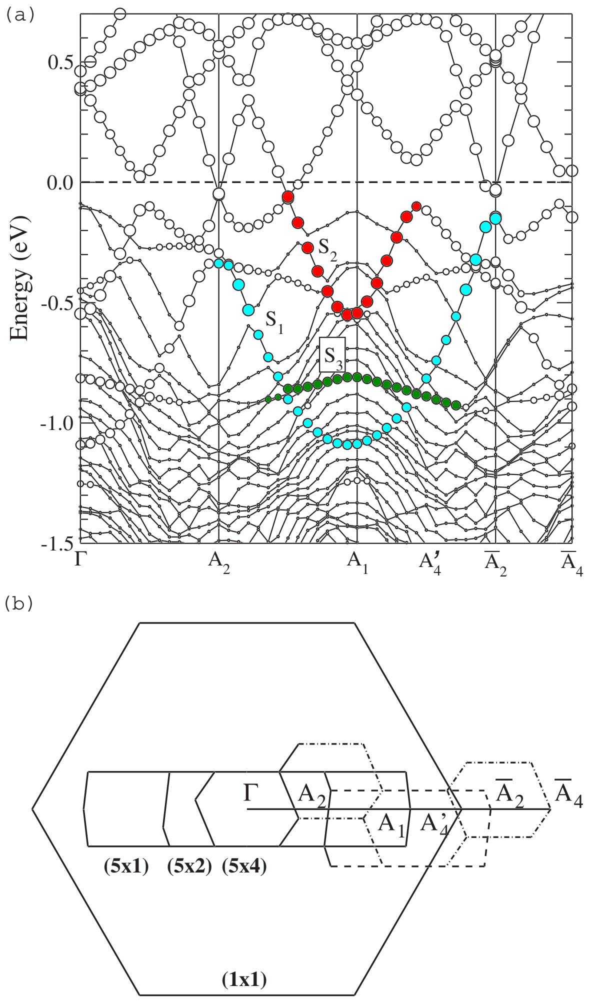

FIG. 2. (Color online) (a) Band structure of the Riikonen and Sánchez-Portal 5×1 model along the gold chain direction. The size of each circle indicates the surface character of the states in the charge around surface-layer atoms. (b) Bidimensional Brillouin zone associated with the 5×1, 5×2, and 5×4 supercells of the Si(111)-Au surface.

nal RS (5×2) model is unstable, but just a shallow energy minimum near its 5×1 variant under the bare local density approximation (LDA). It is found that this model is not even attainable within the GGA scheme. In both GGA and LDA, the RS (5×2) structure is always relaxed to the RS (5×1) by the steepest-decent conjugate-gradient approach. The feature of the asymmetric rise of the silicon atoms is only achieved using the non-steepest-decent quasi-Newton approach under the LDA.

Instead, we attempt to make the periodicity of RS (5×1) doubled to 5×2 by removal of *one* silicon atom per 5×2 unit cell, similar to the treatment in the Erwin case. Surface energies are calculated for removing one silicon atom from all possible sites on the adatom-free surface. The most favorable structure is shown in Fig. 1. Remarkably, Fig. 1 shows that the HC feature in the E or RS models is significantly deformed here after full relaxation. The resultant surface energy compares favorably with that of the $E(5\times2)$ model, being only a minor amount of 1.14 meV/Å^2 higher. (See Note added in proof.) This is due to the fact that, in the Erwin model, removing certain silicon atoms plays an additional role in diminishing the overcoordination of other silicon atoms.[38]

Figure 3(a) depicts the band structure of the present model. The main surface bands in Fig. 2(a) also appear in this figure. Of particular importance is the surface band S_2 just below E_F, which agrees broadly with the ARPES data.[32,33] Similar to the earlier calculations,[39] the dispersive S_1 and S_2 bands mostly originate from the interaction between the two gold rows and the silicon atoms between them. Photoemission data reveal that the dispersion of the S_1 band changes from one dimensional near the band maximum (A_2) to two dimensional near its minimum[31] (A_1) and the S_2 band behaves as one dimensional[32,33] near E_F, especially at the 5×4 boundaries.[33] The right panels of Fig. 3(a) indicate that the perpendicular dispersions at the top of the S_1 band and its bottom are 0.01 and 0.05 eV, respectively, comparable to the experimental values[31] of 0.03±0.03 and 0.14±0.03 eV. The calculated perpendicular dispersion of the S_2 band near the Fermi level at one of the 5×4 boundaries, A_4', is also presented in the extreme right panel for comparison.

Away from the protrusions, filled-state experimental STM images for the Si(111)-(5×2)-Au surface show an array of Y-shaped features with 5×2 periodicity. The Y-shaped feature is composed of one "V head" and one bright tail, with a well-defined crystallographic orientation with respect to the underlying substrate.[20–22] The STM simulation image of the present 5×2 model with no adatoms is shown in Fig. 3(b). They were obtained in an intercepted plane 1.5 Å above the gold rows by integrating the charge density from $E_F - 0.8$ eV to E_F. A probable Y-shaped feature with the correct orientation could be identified in this figure.

We now consider the role of the adatoms decorated in the underlying 5×2 surface. A recent STM study[28] and theoretical calculations[38] strongly suggest that the BPs should be Si adatoms. The present calculations also show that, when extra Au atoms are located at several possible testing sites, they relax well into the surface layer and thus produce no detectable STM spot. We, therefore, make no further consideration of Au as a candidate for the BPs in the discussion below. To determine the location of the Si adatom, all possible sites of the parent 5×2 surface are energetically examined. The most favorable site is shown in Fig. 1. The height of the adatom is estimated as 1.2 Å relative to the "background" along the gold chain, consistent with the work in Ref. 26. Based on this result, we further explicitly perform the total-energy calculations for one adatom per 5×4 and 5×6 supercells, equal to the adatom coverage x of 1/2 and 1/3, respectively. The corresponding surface energies are compiled in Table I. It is shown that the surface energy will increase when Si adatoms occupy every 5×2 unit cell.[43] However, in the situation of one adatom per two 5×2 unit cells, the energy is dramatically lowered by 1.87 meV/Å^2 and is very close to the Erwin case (within 0.42 meV/Å^2 only[44]). Most importantly, the situation with this optimal adatom coverage is more stable than the adatom-free structure by a 0.49 meV/Å^2 lowering of the surface energy, reflecting the natural existence of the BPs on the surface. The

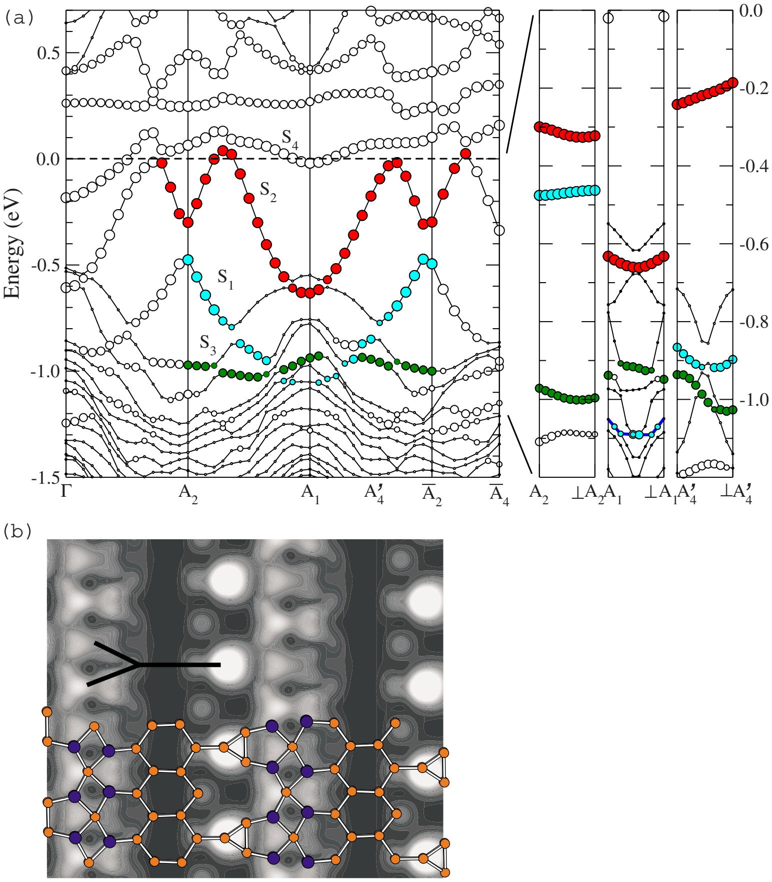

FIG. 3. (Color online) Band structure and STM image of the present adatom-free model. (a) Left and right panels show the band structures along and perpendicular to the gold chain direction, respectively. Note the change of the energy scale. The meaning of each circle is described in Fig. 2(a). (b) Simulated STM image under a sample bias of −0.8 eV.

almost negligible energy difference between the cases of $x=1/2$ and $1/3$ implies sufficient room in the 5×4 supercell for the full relaxation of the silicon adatom. As a result, the interaction between the BPs with 5×4 periodicity could be rather weak, giving rise to the observed random lengths of BP chains. However, there should be at least one adatom-free 5×2 segment between the BP chains shown above. Hence, these calculations are consistent with the experimental observations.[25–28] The mechanism of the random distribution of BPs is investigated in more detail based on the lattice fluid of Si adatoms.[27]

We first present in Fig. 4 the band structure of the Si(111)-(5×2)-Au surface with one Si adatom per 5×2 cell ($x=1$). Obviously, the addition of Si adatoms renders the full system insulating. The adatom supplies electrons to dope the S_2 and S_4 bands of the undecorated surface and push these bands below E_F. As expected, Fig. 5(a) shows smaller shifts of these two bands for the $x=1/2$ case (here, the smallest circles are dropped out and the color of the solid lines is modified for better illustration). Consequently, the chain structure converts from metallic to insulating through the existence of the S_2 and S_4 bands doped by extra Si adatoms. The present model, indeed, shows that the 5×2 adatom-free "section" is metallic and the 5×4 adatom section is insulat-

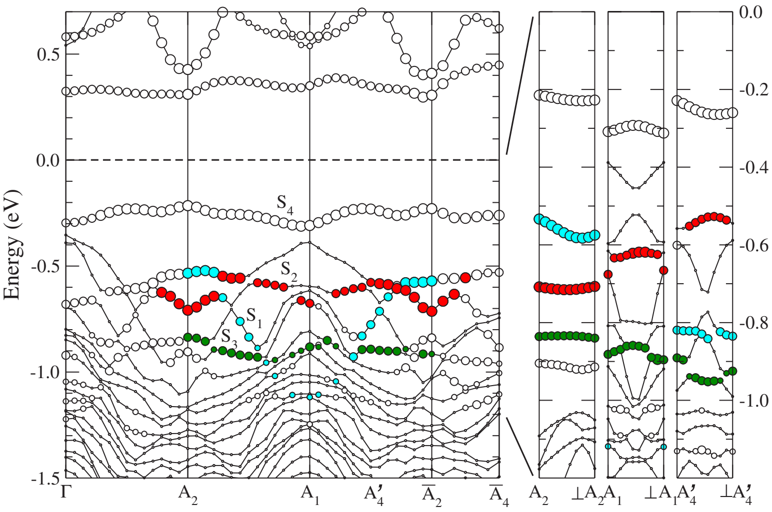

FIG. 4. (Color online) Band structure of the present model decorated with one Si adatom per 5×2 cell. The same drawing schemes as in Fig. 3(a) are used.

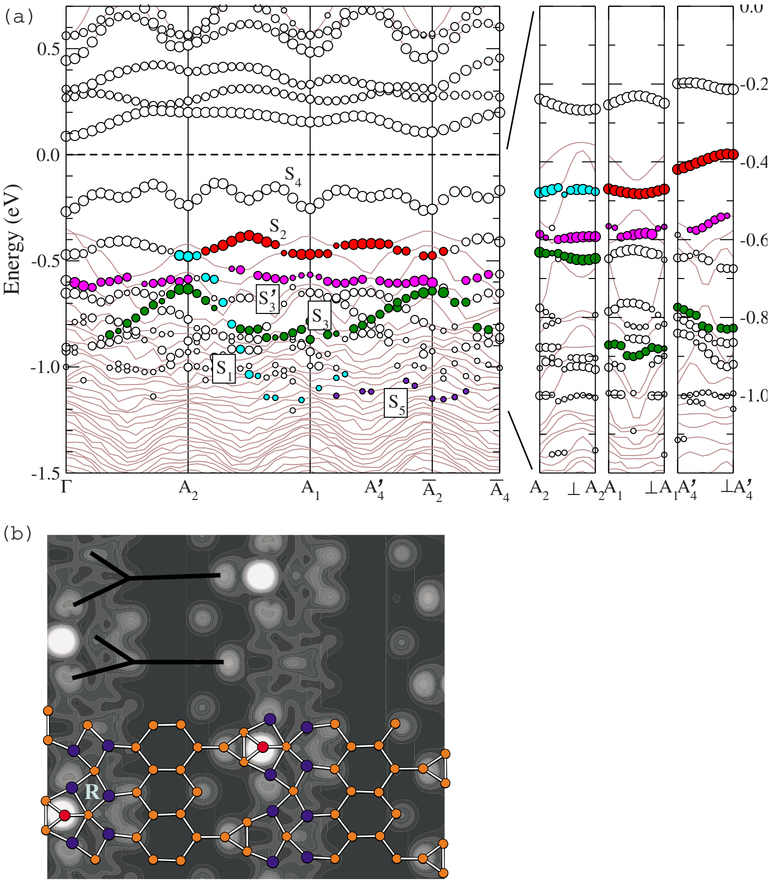

FIG. 5. (Color online) Band structure and STM image of the present model with one Si adatom per two 5×2 cells. (a) The same drawing schemes as in Fig. 3(a) are used. Here, the smallest circles are dropped out and the color of the solid lines is modified for better illustration. (b) Simulated STM image under a sample bias of -0.8 eV.

ing, in agreement with recent findings.[22,33] Particularly, when compared with Fig. 4, Fig. 5(a) shows an additional S_3' band, which is also identified in the experimental data.[32] It is found that the calculated band structure of the $x=1/2$ case is in overall agreement with the experiment by Matsuda *et al.*[32] Note that the "surface" character of the S_5 band and the bottom of the S_1 band will be enhanced if the contribution of the silicon layer just below the surface layer (colored in Fig. 1) is taken into account. As for the situation perpendicular to the gold chains, the band dispersions at the zone boundaries are more or less similar to those of the surface without adatoms. It is worthy pointing out that, as shown in Fig. 5(a), the perpendicular dispersion of the S_4 band at A_4' is only 0.02 eV, indicating the one-dimensional character of this band near E_F.[32,33]

Figure 5(b) demonstrates the STM image for a 5×4 arrangement of the extra adatom, corresponding to the concentration that could actually be reached in the experiment. Clearly, the figure shows the very pronounced bright protrusions due to the silicon adatoms. More detailedly, these BPs are located near the V-head portions of the Y-shaped features, consistent with a very recent STM experiment.[25] However, the BPs were found experimentally to be symmetrical[25] rather than, in this work, off-symmetrical between adjacent V heads. Regardless of the cost of a higher surface energy, we examined the possibility of relocating the adatom to the more symmetrical neighboring site marked *R* in Fig. 5(b). Nevertheless, the final results indicate that, in the case of $x=1/2$, the adatom is merged into the surface layer due to the diffusion of the neighboring Au atoms toward the vacant positions left by the removed silicon atoms. The increase in the surface energy is significantly too large (2.5 eV per 5×2 cell or 19 meV/Å^2) to directly rule out this resultant atomic structure. Further theoretical and experimental work will be needed to completely clarify this issue.

In summary, we have proposed an alternative model for the Si(111)-(5×2)-Au surface reconstruction. This model is energetically very competitive with the Erwin model.[38] Simulated STM images of the present model reproduce a clear series of Y-shaped features with correction orientation as well as the so-called bright protrusions due to the Si adatoms. In addition to the predominant surface band S_1 between the 5×2 and 5×1 boundaries, the band structure calculations also show another surface band S_2 very near E_F, which is closely related to the debate of whether the Si(111)-(5×2)-Au surface is metallic or not.[22,32,33] The decoration of the adatom on the parent adatom-free surface supplies electrons to dope the S_2 band and changes the system from metallic to insulating, consistent with the recently observed phase separation.[22,33] The finer-level phenomena of the continuous transition from one-dimensional behavior at the top of the S_1 band to two-dimensional behavior at its bottom,[31] and the one-dimensional character of the weaker S_2 band at the 5×4 boundaries,[33] are also accounted for in this model. Finally, the occupation of the Si adatom is found to be at most one adatom per two 5×2 unit cells, in agreement with experiments.[25–28]

Note added in proof. Recently, we recalculated the surface energies of the $x=0$ and 1 cases with the more dense grid of 2×6 for the BZ sampling. It was found that the resultant surface energy of the present model with no adatoms was only 0.29 meV/Å^2 higher than that of the Erwin model. There was no significant change in the surface energies of the $x=1$ cases.

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*Corresponding author; cyren@nknu.edu.tw

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[43] In the Erwin case, the effect of Si adatoms surface energies behaves differently in our GGA and LDA calculations. The latter yields a decrease of 1.5 meV/Å^2 in the surface energy with one Si adatom per 5×2 cell, in agreement with previous results (Ref. 39).

[44] This is near the limiting precision inherent to one-particle DFT calculations.