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Doping of the step-edge Si chain: Ag on a Si(557)-Au surface

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Structural and electronic properties of monatomic Ag chains on the Au-induced, highly ordered Si(557) surface are investigated by scanning tunneling microscopy (STM)/spectroscopy and first-principles density functional theory (DFT) calculations. The STM topography data show that a small amount of Ag (0.25 ML) very weakly modifies the one-dimensional structure induced by Au atoms. However, the bias-dependent STM topography and spectroscopy point to the importance of the electronic effects in this system, which are further corroborated by the DFT calculations. The obtained results suggest that Ag atoms act as electron donors leaving the geometry of the surface almost unchanged.

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I. INTRODUCTION

One-dimensional (1D) metallic structures can be fabricated on stepped semiconductor surfaces and used to study the electronic properties of electrons confined to a single spatial dimension.[1–5] The most straightforward approach to create the 1D structures is a process of self-assembling of atoms on stepped semiconductor surfaces. The gold-decorated Si(557) surface is one of such systems.[6] It consists of the Si(111) terraces $5\frac{2}{3}\times a_{[11\bar{2}]}=1.92$ nm wide and is tilted 9.5° toward the $[\bar{1}\bar{1}2]$ direction. Deposition of 0.2 monolayer (ML) of Au (1 ML corresponds to 7.83×10^{14} atoms/cm^2) stabilizes this surface[6] with a regular array of two nonequivalent chains per terrace.[2,6–10]

The fact that the interchain spacing is large, due to wide (1.92 nm) terraces of the Si(557)-Au surface, is reflected in very weak interchain coupling so the surface is almost perfectly 1D. Therefore this surface has attracted much attention in relation to the characteristic phenomena for 1D systems, like the Luttinger liquid (LL) or the Peierls metal-insulator transition.[11] Indeed, Segovia *et al.*[12] reported the angle-resolved photoemission spectroscopy (ARPES) data of the Si(557)-Au surface. They observed two bands which seemed to merge into a single peak at the Fermi energy (E_F)—a typical behavior characteristic for the LL state. Later the ARPES studies with a better resolution have not confirmed the existence of the LL, and the measured band-structure features two proximal bands crossing the E_F.[13–15] Note, however, that the electron energy-loss spectroscopy measurements[16] indicated a significant role of the electron correlations in this system. Those proximal bands have been assigned to two different types of chains on the surface.[13,14] Moreover, Ahn *et al.*[14] showed that at the room temperature (RT) one of the bands is insulating and the other one is metallic, and the metallic band undergoes the Peierls metal-insulator transition at low temperatures. However, very recent ARPES measurements[15] indicate that both bands are metallic at the RT and have nearly identical behavior with the temperature. This has been confirmed by the density functional theory (DFT) calculations,[17,18] according to which two proximal bands observed in the ARPES experiments come from the Rashba spin-orbit splitting of the band associated with the Si-Au bonds.

Scanning tunneling microscopy (STM) images reveal two nonequivalent atomic chains on each terrace parallel to the step edges with occasional bright protrusions on top of the chains.[2,9,13,14,19,20] One atomic chain, which dominates in the empty-state STM images, appears to be insulating at the RT (Ref. 19) and is comprised of the Si adatoms located in the middle of terrace.[2,17,18] The second chain, dominating in the filled-state STM images, is metallic at the RT (Ref. 19) and originates from the dangling bonds of the step-edge Si atoms.[2,17,18] Both chains show the periodicity doubling along the terraces, and the step-edge Si atoms chain shows the reversed STM topography when the sample bias polarization is changed.[9] The topography reversal has been explained it terms of the buckling of the step-edge Si atoms,[18,20] which was also observed in the case of the Si(335)-Au and Si(335)-Au/Pb systems.[21] At low temperature, the system lowers its energy by freezing every second step-edge Si atom in the up (down) position. As a consequence of that the up-edge (down-edge) Si atoms feature the fully occupied (empty) dangling bonds. Measuring the STM topography we observe the up-edge at the negative polarization and the down-edge at the positive polarization. Thus, the buckling explains the observed STM topography reversal. Note that the second chain comprised of the Si adatoms does not show any buckling, and no topography reversal is observed,[18] in full agreement with the experimental data.[9]

On the other hand, silver deposited on the vicinal Si surfaces also leads to the 1D chain structures and elongated islands.[22–28] In particular, the STM topography of the Si(557) surface covered with 0.2 ML of Ag and annealed shows the atomic chains separated by 5.73 nm, i.e., three times the width of an ideal Si(557) terrace.[26,27] So the surface looks more like the bare Si(557) surface[29] than the Si(557)-Au surface.[2,9,13,14,19,20] Note that the bare Si(557) surface features the (111)7×7 terraces separated by the triple-height steps. On the Ag-modified Si(557) surface, the 7×7 reconstruction is changed into the chain structure, and the rows of atoms are believed to be the Si adatoms.[26,27] Thus, the Si(557)-Ag surface shows the features characteristic of the bare Si(557) surface (triple terraces) as well as of the Si(557)-Au surface (chains of the Si adatoms).

To shed some light on the behavior of Ag on the Au-induced vicinal Si surfaces, we present here an experimental and theoretical study of the submonolayer coverage Ag deposited on the well-ordered Si(557)-Au surface. Some preliminary results, regarding the Ag coverage (0.25–1.8 ML) dependent morphology of the surface and the effect of annealing on the resulting surface, have been published in Ref. 28. Here we focus on the structural and electronic properties of the Si(557)-Au surface covered with 0.25 ML of Ag, examined by the STM and scanning tunneling spectroscopy (STS) supplemented by the DFT calculations. Our STM study shows that 0.25 ML of Ag modifies rather weakly the topography of the surface, and the main features of the Si(557)-Au surface, i.e., the double chain structures are still observed. The DFT calculations show two nonequivalent positions of the Ag adsorption, one at the step edge and the other one in the middle of terrace. The simulated STM images based on the obtained structural model as well as the calculated local density of states agree well with the experimental STM and STS data. Our results suggest that it is possible to electron dope the original Si(557)-Au surface without any substantial structural modifications of it, similar as in the case of flat Si surfaces, like Si(111)5×2-Au where the surface was doped by extra Si adatoms[30] or the Si(111)4×1-In surface doped by Na atoms.[31] This opens a route to change the electronic properties of the one-dimensional objects fabricated on stepped Si surfaces almost without modifications of the structure.

The rest of the paper is organized as follows. The details of the experiment and the calculations are presented in Secs. II and III, respectively. Section IV contains the STM topography results. The proposed structural model together with the simulated STM images of the surface are presented and discussed in Sec. V while Sec. VI is devoted to the electronic properties of the surface. Finally, some conclusions are drawn in Sec. VII.

II. EXPERIMENT

The scanning tunneling microscopy and spectroscopy experiments were performed in an ultrahigh-vacuum system which was equipped with the Omicron VT STM and the reflection high-energy electron diffraction (RHEED) system. The base pressure was 5×10^{-11} mbar. The substrates were *n*-type Si(557) wafers with about 1 Ω cm resistivity at the room temperature and dimension $10\times 1.5\times 0.4$ mm^3. Cleaning was performed in the vacuum by flashing for few seconds to around 1550 K under the RHEED control, which produced a clean surface without SiC contamination. Direct resistive heating of the Si crystal was used. The ordered surface in the form of the one-dimensional structures has been obtained after the deposition of 0.2 ML of Au, heating the sample at temperature 950 K for 20 s and gradually annealing to the room temperature for 3 min. The STM images showed a well-ordered surface with double atomic chains on each 1.92-nm-wide terrace.[9] Ag was evaporated on the Si(557)-Au substrate held at the RT at rate of about 0.1 ML/min. During the deposition of Au and Ag the pressure in the vacuum chamber never rose above 1×10^{-10} mbar. The quartz-crystal monitor was calibrated using the RHEED intensity oscillations during the layer-by-layer growth of Pb on a flat Si(111) substrate.[32] The temperature of the sample with Ag was estimated from the dc flowing through the substrate, using the calibration curve made for a similar bare Si sample.

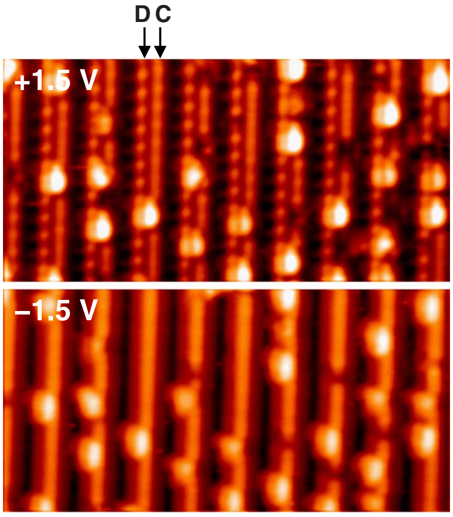

FIG. 1. (Color online) 18×9 nm^2 STM images of the same area of the Si(557)-Au surface recorded at the sample bias +1.5 V (top panel) and −1.5 V (bottom panel). The chain associated with the step-edge Si atoms is denoted by C and the chain composed of the Si adatoms by D.

III. DETAILS OF CALCULATIONS

The calculations have been done using the SIESTA code,[33–37] which performs the standard pseudopotential density functional calculations using a linear combination of numerical atomic orbitals as a basis set. The local density approximation (LDA) to DFT (Ref. 38) and Troullier-Martins norm-conserving pseudopotentials[39] have been used. A double-ζ polarized basis set was used for all the atomic species.[34,35] The radii of the orbitals for different species were following (in a.u.): Ag—4.16 (4*d*), 6.85 (5*s*), and 6.52 (5*s*), Au—7.20 (5*d*), 6.50 (6*s*), and 5.85 (6*p*), Si—7.96 (3*s*), 7.98 (3*p*), and 4.49 (3*d*), and H—7.55 (1*s*) and 2.94 (2*p*). Due to large real-space supercell, only four nonequivalent *k* points for Brillouin-zone sampling and a real-space grid equivalent to a plane-wave cutoff 100 Ry were employed.

The Si(557)-Au/Ag system has been modeled by four silicon double layers and a vacuum region of 19 Å. All the atomic positions were relaxed until the maximum force in any direction was less than 0.04 eV/Å, except the bottom layer. The Si atoms in the bottom layer were fixed at their bulk ideal positions and saturated with hydrogen. To avoid artificial stresses, the lattice constant of Si was fixed at the calculated value, 5.39 Å.

IV. STM TOPOGRAPHY

The topographic STM images of the Si(557)-Au surface before and after the deposition of 0.25 ML of Ag are shown in Figs. 1 and 2, respectively. At first sight both surfaces look similar to each other, i.e., we observe two different chains on each terrace. All the chains have the periodicity along the terraces equal to $2\times a_{[1\bar{1}0]}$, where the $a_{[1\bar{1}0]}$ is the distance

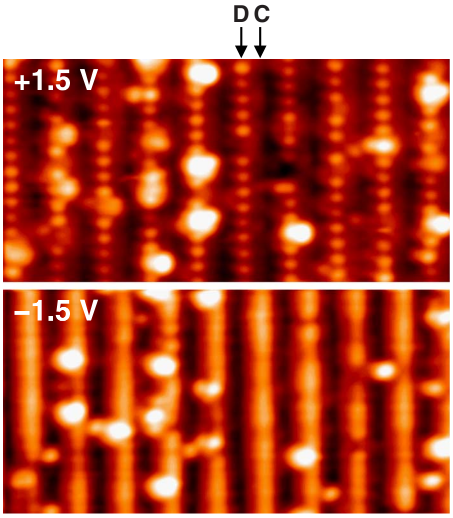

FIG. 2. (Color online) 18×9 nm^2 STM images of the same area of the Si(557)-Au surface covered with 0.25 ML of Ag. The sample bias was +1.5 V (top panel) and −1.5 V (bottom panel).

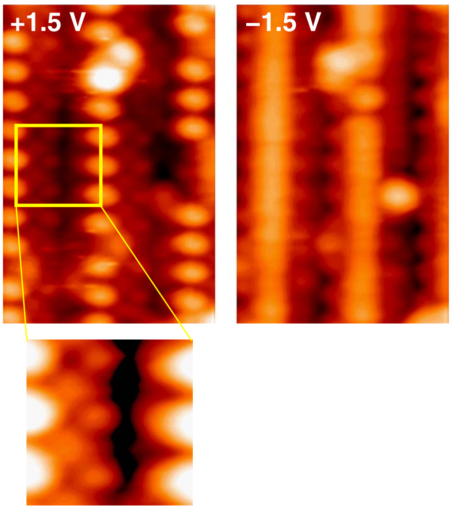

FIG. 3. (Color online) 4.3×8.6 nm^2 STM images of the same area of the Si(557)-Au/Ag surface recorded at $U=+1.5$ V (left panel) and $U=-1.5$ V (right panel). Inset to the figure shows the zoom-in of the zigzag structure marked in the left panel.

between the Si atoms in $[1\bar{1}0]$ direction. As it was mentioned already, in the case of the Si(557)-Au surface, the continuous (C) chain comes from the step-edge Si atoms while the discontinuous (D) one is due to the Si adatoms in the middle of terrace. On the other hand, the deposition of Ag on the Si(557)-Au surface modifies slightly the STM topography. We observe the chain C at the negative sample bias and the chain D at the positive polarization. Note that in the case of the Si(557)-Au surface a pair of chains (C and D) is observed at both polarizations. Here, on the Si(557)-Au/Ag surface, we observe only single chain at a given polarization.

A close resemblance of those structures can suggest that either the Ag atoms are for some reason invisible to the STM or they adsorb at the step edges, thus the positions of all the steps are slightly shifted, and the STM topography remains almost unchanged. To see which of two scenarios is realized in experiment, we have measured the distance between the chain C (step edge) and the chain D (Si adatoms) in the case of the Si(557)-Au and the Si(557)-Au/Ag surfaces. It turns out that the measured distance is the same in both cases (within the estimated error), and equal to 0.64 nm, so we can conclude that on the Si(557)-Au/Ag surface we also observe the step-edge Si atoms (chain C) and the Si adatoms (chain D). The Ag atoms seem to be invisible to the STM. A closer inspection of the STM data reveals that the Ag atoms modify the topography of the surface, especially at the positive polarization (see Fig. 3). The empty-state STM topography (left panel of Fig. 3) shows the chain D and a zigzag structure (see inset of Fig. 3) in place of the chain C (visible in the right panel). Note that in the case of the Si(557)-Au surface the chain C is also visible at the positive polarization. Comparing the empty-state topographs of both surfaces, we can conclude that the zigzag structure is due to the step-edge Si atoms and the Ag atoms adsorbed at the step edge. The filled-state STM topography (right panel of Fig. 3) looks very similar to the Si(557)-Au surface with the chain C and less visible chain D. As we already mentioned the distance between the chains C and D does not change after the deposition of Ag, so we can conclude that chain C is now also due to the step-edge Si atoms. Thus the Ag atoms adsorbed at the step edge act as electron donor, supplying the step-edge Si atoms with the electrons. Therefore the step-edge Ag atoms are invisible in the filled state but appear in the empty-state STM topography. To further check the validity of our picture we have performed the DFT calculations and propose the structural model which supports our conclusions.

V. STRUCTURAL MODEL AND STM SIMULATIONS

In search for the lowest energy structural model of the Si(557)-Au/Ag surface we have taken two Ag atoms per the unit cell (see Fig. 4), which is close to the experimental value of 0.25 ML of Ag. Based on the experimental conditions, we have also assumed that the Ag atoms adsorb at the surface, and they do not substitute for the surface layer atoms. Out of 260 structural models investigated, the most stable structural model of the Si(557)-Au/Ag surface is shown in Fig. 4. The Ag atoms form two chains, one at the step edge and the other one on the terrace. The step-edge Ag atoms are bonded to two step-edge Si atoms while the atoms in the middle terrace Ag chain are bonded to the Au chain and to some of the honeycomb chain (HC) Si atoms. Note that the HC structure is a common feature of all the vicinal Si surfaces.[2,17,18,21,40,41] The distance between the Ag atoms in both chains, similar as the distance between the Si adatoms, is equal to $2\times a_{[1\bar{1}0]}$.

At this point we would like to comment on the other structural models. The next "best" structural model has the surface energy only 0.1 meV/Å^2 [15 meV per the Si(557)2×1 unit cell shown in Fig. 4] higher than the model shown in Fig. 4 and is very similar to it. The difference is the positions of the middle terrace Ag atoms, which are shifted by single lattice constant in the direction $[1\bar{1}0]$. Both models have very similar properties, and the differences are rather subtle. Moreover, since in the experiment we observe the

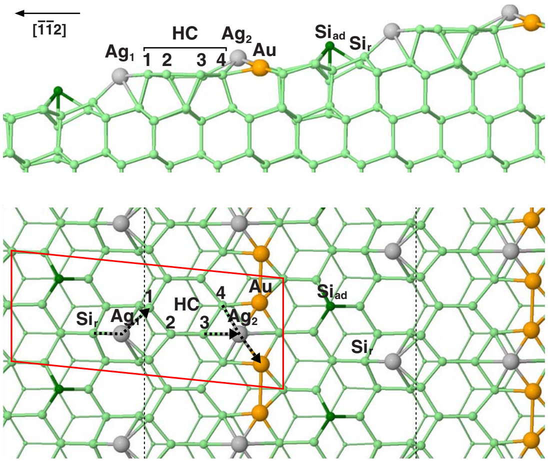

FIG. 4. (Color online) Structural model of the Si(557)-Au/Ag surface. Top panel shows side view of the structure and the bottom panel top view with marked surface unit cell. The second uppermost Si double layer is also shown in the bottom panel. Different colors reflect different species of the structure: Si atoms (adatoms)—small light (dark) green circles, Au atoms—large yellow circles, and Ag atoms—large silver circles. Labels 1–4 stand for the Si atoms forming the HC, Si$_{ad}$ and Si$_r$—silicon adatoms and restatoms while Au and Ag$_1$ (Ag$_2$) stand for gold and silver, respectively. Black dashed lines with arrows indicate the paths along which the valence charge redistribution were calculated (see Fig. 6).

features associated with the step edge and with the Si adatoms, it would be very hard to determine which of two models corresponds to the experimental situation. Such a small energy difference between those models allows us to expect that both models are likely to be realized. Another structural model, with the surface energy higher by 1.8 meV/Å^2 (252 meV per unit cell), features the single Ag chain only located at the step edge with the Ag atoms separated by single lattice constant in the direction [1$\bar{1}$0], thus disagree with the STM topography data. The remaining models have much higher surface energies.

Having the structural model of the Si(557)-Au/Ag surface featuring two Ag chains, it is natural to ask which of two different kinds of the adsorption sites becomes populated first, the step edge (Ag$_1$ in Fig. 4) or the Au chain (Ag$_2$). To answer this question, we have performed the DFT calculations for two times lower Ag coverage, i.e., a single Ag atom per two unit cells. The obtained results suggest that the adsorption energies at the step edge and at the Au chain are almost degenerate. To be more precise, the adsorption energy at the Au chain is by 0.3 meV/Å^2 (46 meV per unit cell) lower comparing to the step-edge site. Thus, we can expect that both chains appear simultaneously.

Comparing the present most stable structural model (Fig. 4) with the model of the Si(557)-Au surface (see Refs. 2, 17, and 18) one can notice that the Ag atoms almost do not modify the original Si(557)-Au surface. This confirms the conclusions derived from the STM measurements.

To check the validity of the present model against the STM topography data, we have performed the STM simulations within the Tersoff-Hamann approach.[42] The results of the empty- and the filled-state constant current topography are shown in Fig. 5. At positive sample bias we observe the bright spots associated with the Si adatoms (chain D) and the zigzag chain, and at negative bias—the chain corresponding to the step edge (chain C) and less visible chain D, in full agreement with the experimental data (compare Fig. 3). Comparing the empty-state image with the structural model shown in the top of the Fig. 5, one can notice that the zigzag chain comes from the step-edge Ag atoms and some of the Si atoms forming the HC structure. On the other hand, the chain C visible in the filled-state image is associated with the step-edge Si atoms. The calculated distance between those chains is equal to 0.63 nm, which is very close to the experimental value of 0.64 nm and is the same as in the case of the Si(557)-Au surface. All the above clearly demonstrates that the Ag atoms act as electron donor, which supply the step-edge Si atoms with extra electrons, as was suggested in Sec. IV.

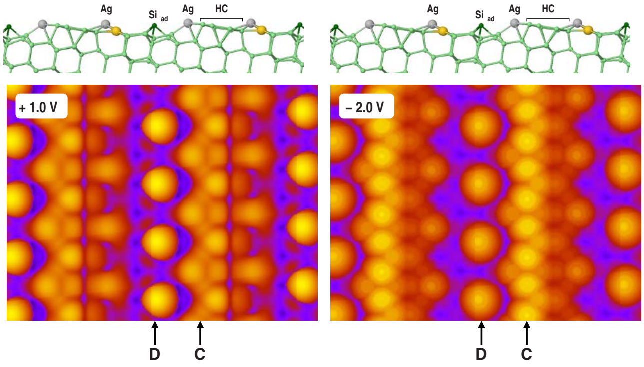

FIG. 5. (Color online) Empty-state (left panel) and filled-state (right panel) STM simulations of 4.1×3.1 nm^2 area of the Si(557)-Au/Ag surface. The side views of the present structural model are shown on top of the figure.

To further corroborate the doping scenario we have calculated the difference of the valence charge $\Delta\rho$ defined as the valence charge of the structure minus the atomic valence charge ($\Delta\rho=\rho-\rho_{atm}$) along some characteristic paths indicated in Fig. 4. The results are presented in Fig. 6. Panel (a) shows the $\Delta\rho$ calculated along the path starting at the position of the Si restatom Si$_r$ through the step-edge Ag atom to the HC$_1$ Si atom (see Fig. 4). Clearly, the electron charge is transferred from the Ag atom to neighboring the step edge and the restatoms. Similar behavior shows the Ag atom located in the middle of terrace which give away the electron charge to the HC$_3$ and HC$_4$ atoms, as illustrated by solid and dashed lines in Fig. 6(b), respectively.

The above discussion clearly indicates that the experimental STM data can be satisfactorily explained in terms of the step-edge Si chain doping by the adsorbed Ag atoms.

VI. ELECTRONIC PROPERTIES

To shed additional light on the electronic properties of the Si(557)-Au/Ag surface we have performed the spectroscopy (STS) measurements, which in first approximation is a measure of the local density of states (LDOS). The normalized differential conductance data recorded at different surface

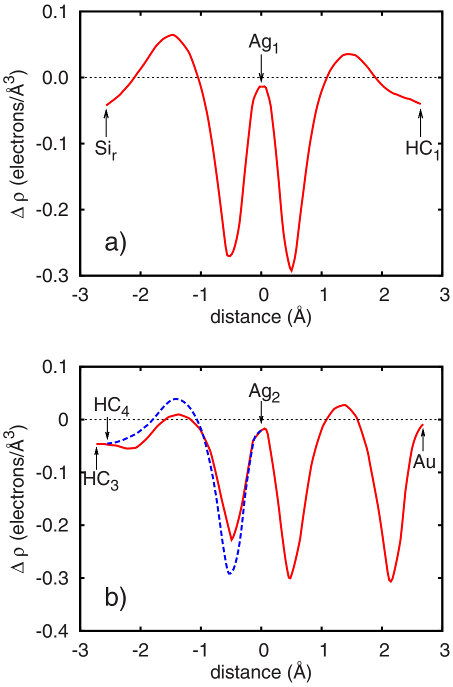

FIG. 6. (Color online) The valence charge difference $\Delta\rho$ defined as the valence charge minus the atomic valence charge ($\Delta\rho=\rho-\rho_{atm}$). Panel (a) shows the $\Delta\rho$ calculated along the path Si$_r$-Ag$_1$-HC$_1$, i.e., passing through the step-edge Ag atom while panel (b)—along the paths containing the middle terrace Ag atom: HC$_3$-Ag$_2$-Au (solid line) and HC$_4$-Ag$_2$ (dashed line). For labeling see Fig. 4, where also the paths are indicated.

regions are shown in Fig. 7. Each point of the differential conductance represents the average over 60 $I(V)$ curves which have been numerically differentiated.

The main features of the characteristics shown in Fig. 7 are the energy states around −0.5 and +1.0 V for the HC structure, around −0.6 and +0.8 V for the Ag chain, around +0.3 and +0.8 V for the Si$_{ad}$ chain. Note that at negative voltages, the normalized conductance of the Si$_{ad}$ chain shows almost featureless and increasing behavior.

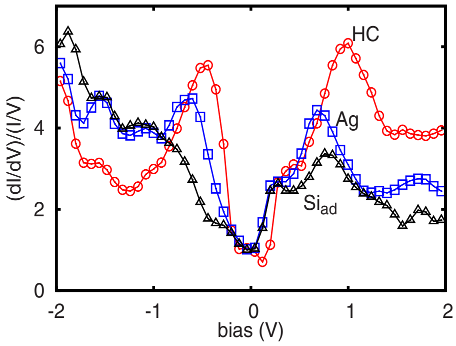

FIG. 7. (Color online) Scanning tunneling spectroscopy of various regions the Si(557)-Au/Ag surface. The HC curve represents the STS recorded at the HC structure near the step edge, Ag—at the Ag chain while Si$_{ad}$—the characteristics taken over the Si adatoms. Compare Fig. 4.

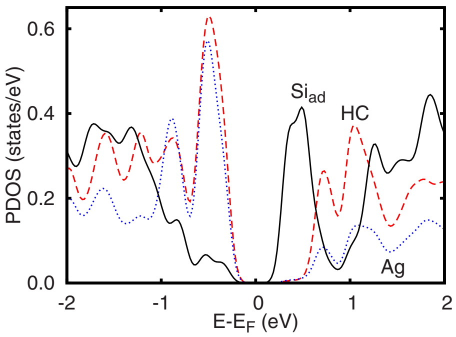

FIG. 8. (Color online) PDOS of the atoms forming the different structures indicated in the figure.

We have also calculated the projected density of states (PDOS) of the atoms located in corresponding regions of the Si(557)-Au/Ag surface, which can be compared to the STS data of Fig. 7. The PDOS of the atoms forming the HC, the Ag chain (Ag) and the Si adatom chain (Si$_{ad}$) are shown in Fig. 8. Clearly, one can see a good qualitative agreement with the spectroscopy data, presented in Fig. 7. In particular, we observe the energy peaks around 0.5–0.6 eV below the Fermi energy for the HC and Ag chains and almost featureless the filled-state PDOS for the Si$_{ad}$ chain. We can also notice some similarities between PDOS and the STS spectra in the empty-state regime, in particular the states around +0.8 and +1.0 eV for the HC and the Ag chains. However, due to the known limitations of the DFT theory above the Fermi level, those results should be taken with caution. Nevertheless, the filled-state PDOS agrees well with the measured STS characteristics.

To further confirm the validity of the scenario of the step-edge electron doping by the Ag atoms, we focus on the shifts of the main Si-related features in the PDOS and in the band structure with respect to the Fermi energy. The comparison of the PDOS of different surface atoms in the case of the Ag and Ag-free the Si(557)-Au surface is shown in Fig. 9. It is clearly seen that the adsorbed Ag atoms shift the main features (indicated by arrows) of different atoms. What is more important, the shifts of the states are different for different atoms. This comes from the fact that the surface is not doped as a whole but locally by single Ag atoms. Since we have the Ag atoms adsorbed in two nonequivalent sites, we can expect the strongest charge transfer from the Ag atoms to neighboring surface atoms, and thus larger shifts of their electronic states. The most shifted state is that of the down-edge Si atoms, as indicated by arrow in panel (a). The shift of this state is as large as 0.65 eV toward the lower energies. On the other hand, the up-edge Si atom state is not affected by the Ag atoms. This can be understood as follows. As it was discussed in Sec. I, the Si(557)-Au surface features the buckling of the step edge.[18] This mechanism leads to the different occupations of the dangling bonds of the step-edge Si atoms. Originally half-filled step-edge Si bands become empty (down-edge Si atoms) and fully occupied (up-edge Si atoms). Thus only the down-edge Si state can be populated by extra electrons while the up-edge state is already blocked for them. The presence of Ag atoms at the step edge fills the down-edge Si state, thus lowering its energy, and leaves the up-edge Si state unaffected, as is illustrated in panels (a) and (b) of Fig. 9. The electronic states of other surface atoms are

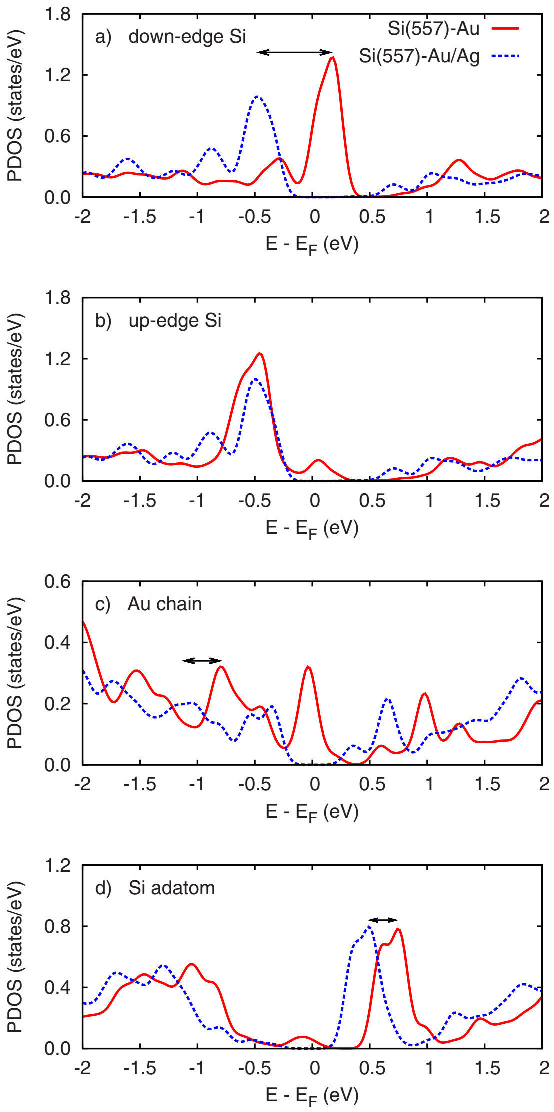

FIG. 9. (Color online) The comparison of the projected density of states between the Si(557)-Au (solid lines) and the Si(557)-Au/Ag surfaces (dashed line). Panel (a) shows the PDOS of the down-edge Si atoms, (b)—up-edge Si atoms, (c)—the Au chain, while (d)—the Si adatoms. The arrows indicate the shifts of the main features due to the adsorption of Ag.

also affected by the adsorbed Ag atoms, albeit more weakly. For example, the bottom of the Au-Si band is moved down by 0.34 eV [see panel (c) of Fig. 9] due to the Ag atoms adsorbed near the Au chain. Similar, the state associated with the Si adatoms is shifted by 0.26 eV [panel (d) of Fig. 9]. Among those atoms, the Si adatoms are the most weakly affected by the adsorption of Ag, since the Ag adsorption sites are far away from the Si adatoms.

All the above discussed effects also are observed in the band structure, shown in Fig. 10. Different symbols reflect the different character of the main surface bands. The bands marked by open circles are associated with the step-edge Si atoms while the filled square bands comes form the hybridization of the Au chain and neighboring surface Si atoms. As it was discussed above, the band associated with the down-edge Si atoms is moved from the Fermi level toward the lower energies and is fully occupied. The presence of the adsorbed Ag atoms near the step edge, almost completely removes the original buckling of the step edge. The difference between the up-edge and the down-edge Si atoms in the z direction is less than 0.1 Å, to be compared with 0.65 Å in the case of the Si(557)-Au surface.[18] As a result both step-edge Si bands are almost degenerate. As it was mentioned previously, other bands are also shifted in the presence of the Ag atoms. The bottom of the Au-Si band (filled squares in Fig. 10) is also moved down by 0.34 eV. What is more important, the charge transfer from the Ag atoms to the Au chain opens a gap in this band. The magnitude of this gap is estimated to be around 150 meV. Probably, in real system this gap will be larger as the LDA always underestimates the band gaps. Nevertheless, the Ag atoms drive the system into insulating state. Note that similar effect of the band-gap opening, associated with the adsorption of the Ag, albeit on the bare Si(557) surface, has been observed.[27] Thus even both surfaces, the bare Si(557) and the Si(557)-Au, feature the different reconstructions, the adsorbed Ag atoms have similar effect on the electronic properties leading to the metal-insulator transition.

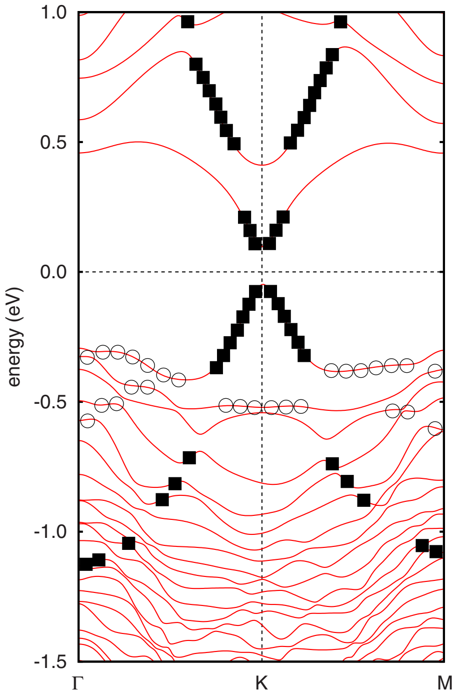

FIG. 10. (Color online) The band structure of the Si(557)-Au/Ag surface, calculated for the structural model shown in Fig. 4. The direction Γ-K-M is parallel to the step edges. The bands marked by open circles are the surface bands of the step-edge Si atoms while the band marked by filled squares comes form the hybridization of the Au and neighboring Si surface atoms.

All the above results fully support the scenario of the doping of the Si(557)-Au surface, mainly the step-edge Si chains, by the adsorption of the Ag atoms.

VII. CONCLUSIONS

In conclusion we have studied the structural and electronic properties of the Si(557)-Au surface covered with Ag atoms. Our STM/STS and the DFT results show that Ag atoms adsorb at the surface and leave the structure of surface almost unchanged, similar as in the case of Ag on the bare Si(557) surface. However, a small amount of Ag (0.25 ML) changes the electronic properties of the Si(557)-Au surface, thus the Ag atoms act as electron donors. In particular, the adsorbed Ag atoms drive the system into insulating state, which could be verified easily in photoemission experiments. In that respect the behavior of Ag on the bare and Au induced the Si(557) surface is similar. Both surfaces become insulating, despite the fact that they feature different reconstructions.

The present study opens a route to electron dope the vicinal Si surfaces without any substantial modifications of the original structure, similar as in the case of flat Si surfaces, like Si(111)5 × 2-Au (Ref. 30) or the Si(111)4 × 1-In surface.[31]

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