Empirical electronic band structure study of silver low–index surfaces

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Abstract
We studied the electronic band structure of the low–index fcc Ag surfaces (001), (110) and (111), by using the empirical tight–binding method in addition with the surface Green function matching method. We report the energy values for different surface and resonance states and compare with the available experimental and theoretical data.
I. INTRODUCTION

In order to predict several surface and bulk crystal properties such as mesoscopic equilibrium shape, surface and catalyst activity [1], growth, creation of rungs and kinks [2, 3], is essential to have a detailed analysis of its electronic band structure. Experimental data is complemented with calculation to obtain a deeply understand of this systems. Two primary types of calculations are used in practice. The first one includes empirical and semi-empirical treatments, from wich empirical tight-binding (ETB) is one of the most transparent and widely used methods, several recent applications of the ETB method can be found in the literature, both for noble metal surfaces [3] and elemental semiconductors [4], as more complex systems like the layered II-IV compunds [5]. The second type are the first-principle calculations based on approximate methods such as density functional theory (DFT), these are located on the most reliable and widely used methods nowadays. In this work the electronic band structures of ideal Ag (001), (110) and (111) surfaces are discussed. This is a continuation of an extensive study of different noble and transition metal surfaces [6].

II. NUMERICAL APPROACH

The ETB calculations were done using a minimal orthogonal basis set. Here, a set of nine “s p d” atomic orbitals per atom in the unit cell were used, and we have included the first nearest and next nearest neighbors as proposed by Papaconstantopoulos [7]. The parameters of the model are those used by Papaconstantopoulos, it is known that these parameters properly reproduce the bulk electronic properties of Ag, according to DFT calculations [7]. To calculate the surface electronic band structure, the Surface Green Function Matching (SGFM) method was used, as suggested by García–Moliner and Velasco [8]. The SGFM method, in conjunction with the ETB approach, was used successfully to study transition metals [9] and semiconductor surfaces [10]. For a complete formulae of the ETB method to the formalism of the SGFM see details in Refs. [8, 10]. A recent application of the method to the study of the electronic structure of different Pt surfaces has been done [11].

From the knowledge of the Green function, the surface and the surface resonances states can be calculated from the poles of the real part of the corresponding Green function. In a similar way, from the imaginary part the local density of states (LDOS) can be obtained.
III. RESULTS AND DISCUSSION

A. Local density of states

Figure 1 shows our calculated LDOS projected on the surface (broken line) and the LDOS projected on the bulk (full line), see figure caption for details.

For the Ag(001) surface a total of 528 k-points were used, here we used the Cunningham method to found the k-point set in the irreducible two dimensional segment of the first Brillouin zone (2D-SBZ) (see inset of Fig. 2(a)) \[12\]. For Ag(110) surface we used 256 Cunningham points in the 2D-SBZ (see inset of Fig. 2(b)). While for the Ag(111) surface we used 136 Cunningham points in the 2D-SBZ (see inset of Fig. 2(c)).

Table I shows the s, p, d atomic orbital partial contribution to the surface and bulk LDOS. A comparison of our calculations with that reported by Papaconstantopoulos \[7\] shows that our method reproduces properly the bulk DOS.

| Surface  | $s_{surf}$ | $p_{surf}$ | $d_{surf}$ | $s_{bulk}$ | $p_{bulk}$ | $d_{bulk}$ |
|----------|------------|------------|------------|------------|------------|------------|
| Ag(001)  | 0.600      | 0.344      | 9.901      | 0.671      | 0.448      | 9.879      |
| Ag(110)  | 0.674      | 0.454      | 9.869      | 0.650      | 0.350      | 10.010     |
| Ag(111)  | 0.670      | 0.440      | 9.870      | 0.650      | 0.350      | 10.010     |

B. Ag (001)

1. Projected bulk electronic band structure, surface– and resonance–states

In an early experimental work Kolb et al. \[13\], by using electroreflectance in the infrared frequency range, reported two surface states (SS) for Ag(001) located in the $\bar{X}$ high symmetry point of the two dimensional Brillouin zone: the first SS was reported at 3.1 eV above the Fermi level, while the second state was reported a few meV below the Fermi level (see Fig. 2 on Ref. \[13\]). In the same work it was found that both states were in good agreement.
FIG. 1: (Color online) Bulk local density of states (LDOS) (black line) and surface LDOS (red line) obtained from the SGFM method. (a) Ag(001)–, (b) Ag(110)–, and (c) Ag(111)–surface. The zero of energies represents the Fermi level.

with ab initio pseudopotential calculations.

Then, Altmann et al. [14] by using angle-resolved Bremsstrahlung isochromat spectroscopy corroborate the states found by Kolb et al. [13] and reported other high energy surface states.

More recently, Savio et al. [15] by using an ab initio pseudopotential calculations combined with ultraviolet photoemission spectroscopy technique refined the previous experimental values for the surface states.

Figure 2 shows our calculated projected bulk band structure and the surface– and resonance–states (RS) obtained from the poles of the real part of the bulk Green function and from the surface Green function, respectively. As we found, there are two SS labeled Es$_1$ and Es$_3$ (full points), and three resonance states labeled Er$_1$, Er$_2$, and Er$_3$ (empty points). The shadow zones represent the calculated bulk band structure projected on the (001) surface. We found that our calculated projected bulk bands are in good agreement with that reported in Refs. [13, 15]. Tables II and III list our calculated energies for the SS and RS found in this work and compare them with other reports. The states $E_{S5}$ and $S_{S6}$ reported in the literature, are listed in Table II although our calculations do not reproduce these states.

2. Detailed discussion of the found SS and RS

As we have found the SS Es$_1$ is located at 4.43 eV at $\bar{\Gamma}$ showing a parabolic dispersion. The state is located in the $\bar{\Gamma}$–gap which has a width of 5.03 eV, approximately, according
FIG. 2: (Color on line) Projected bulk band structure found in our calculation (blue zone). The full (red) points represent the SS, while the empty points are for the RS. (a) Ag(001)–, (b) Ag(110)–, and (c) Ag(111)–surface. The Fermi level is the zero of the energies.

TABLE II: Surface states for Ag(001). The first column is the found SS, the second column list the k-point where the SS was found, the third column shows the experimental energy reported for the related state, the fourth list the theoretical energy value reported in the literature for the SS, the next column shows our calculated energy value for the found SS, finally the last column shows the symmetry of the atomic orbitals that form the SS, according to our calculation. The k–vector is given in units of $\frac{\pi}{a}$, while the energies are in eV.

| SS     | $\vec{k}$ | $E_{\text{exp}}$ | $E_{\text{theo}}$ | $E_{\text{our}}$ | $E_{\text{SFOour}}$ | Symmetry |
|--------|-----------|------------------|------------------|------------------|---------------------|-----------|
| $E_{s1}$ (0,0) | 4.00[14] | 4.43 | $s, p_z$ |
| $E_{s3}$ (1,1) | 0.07[15] | -0.13[13] | 0.96 | $p_x, p_y$ |
| | | -0.15[15] | |
| | | 3.80[17] | |
| $E_{s5}$ (1,1) | 3.50[14] | 3.50[13] | |
| | | 3.03[15] | 2.99[15] |
| $E_{s6}$ (1,1) | -0.53[15] | -0.53[15] | |

to our calculations this state is the hibridization of the $s, p_z$ atomic orbitals. This SS was measured at 4.0 eV by Altmann et al. [14]
TABLE III: Resonance states for the Ag(001) surface. The first column shows the labeled resonance state, the second one shows the wavevector of the state in units of $\frac{\pi}{a}$, the next column shows the related energy in eV, finally the last column shows the wave symmetry found for the different states.

| $E_r$ | $\vec{k}$ | $E_{\text{our}}$ | SFO$\text{our}$ |
|-------|-----------|-----------------|----------------|
| Er$_1$ (2,0) | $-4.06$ | $d_{3z^2-r^2}$ | |
| Er$_2$ (2,0) | $-3.18$ | $d_{xy}$ | |
| Er$_3$ (0,0) | $-4.40$ | $d_{3z^2-r^2}$ | |

We found that the SS $E_{S3}$ is located at 0.96 eV at $\bar{X}$ showing a parabolic dispersion, the state is located in the $\bar{X} -$gap which width is 3.87 eV. We found that this state has the symmetry of the $p_x$, $p_y$ wavefunctions. The state was theoretically reported by Kolb et al. $^{[13]}$, and was recently measured and calculated by Savio et al. $^{[15]}$.

The RS Er$_1$ was found at $-4.06$ eV in the $|\bar{X}\bar{M}|$ direction and shows almost zero dispersion. We conclude that the state is the hybridization of the $d_{3z^2-r^2}$ atomic orbitals.

The RS Er$_2$ begins at $-3.18$ eV in the $\bar{M}$ point showing a small dispersion, as we have found that the character of this state is $d_{xy}$.

The RS Er$_3$ is located at $-4.40$ eV at $\bar{\Gamma}$, the symmetry found for this RS is $d_{3z^2-r^2}$.

The SS’s found in this work for Ag(001) $E_{S1}$ and $E_{S3}$ were reported previously in the literature, and we have found that our calculated energy values for these states show good agreement with published values, as we show in Table II. While the new states found in this work are the resonant states $E_{r1}$, $E_{r2}$, and $E_{r3}$. On the other hand, we do not found the SS $E_{S5}$ and $E_{S6}$ listed in Table II and reported in the Refs. $^{[14, 15, 17]}$.

C. Ag(110)

1. *Projected bulk band structure, surface- and resonance-states*

In an early *ab initio* calculation Ho et al. $^{[16]}$ reported the projected bulk band structure and SS of Ag(110), and predicted a SS on the upper band energy region of the 2D BZ (see Fig. 1(b) in Ref. $^{[16]}$). After that, Reihl et al. $^{[18]}$ using the experimental technique of $k$–resolved inverse photoemission spectroscopy found an unoccupied SS at the energy of
1.65 eV for Ag(110), that matches in good agreement with the state predicted by Ho et al., in the energy gap around the $\bar{X}$ point of the 2D-BZ (see Fig. 2 in Ref. [18]).

Figure 2(b) shows our calculated projected bulk band structure for the Ag(110) surface, which shows eight SS (full points) and six RS (empty points). The details of the calculated surface- and resonance- states are showed in Tables IV and V.

2. Detailed discussion of the found SS and RS

As we found the state $E_{S_1}$, that appears in the upper energy gap located at $\bar{X}$, begins at 5.21 eV and ends at 4.19 eV in the interval $\bar{\Gamma}-\bar{X}-\bar{S}$, crossing the $\bar{X}$ point at 2.89 eV, according to our calculations the state has $p_x$ symmetry of the atomic orbitals. Although there is not experimental evidence for this SS, from a theoretical point of view this state has been reported in the Refs. [13, 16, 19]. We found that the calculated energy for this state is within the reported values (see Table IV).

Moreover, we found another SS in the same gap energy ($E_{S_2}$). The state shows few dispersion, and it is located around 6.2 eV on the $\bar{X}$ point. Our calculated wavefunction for this state has the $s$, $p_z$ symmetry of the atomic orbitals. From the experimental point of view this SS was reported by Altmann et al. [14] and was found around 5.0 ±0.2 eV, while the one calculated by Ho et al., [16] was located at 4.25 eV.

Also, we found that the state $E_{S_3}$ shows a great slope, and it is located in the $\bar{X}-\bar{S}$ interval at energies that range from 8.0–10.0 eV. The wavefunction for this state has the $p_y - p_x$ symmetry of the atomic orbitals. We do not find experimental evidence for this SS, although the state was reported in a theoretical work by Tjeng et al. [19].

The SS $E_{S_5}$ is located at 6.05 eV in the $\bar{S}$ point and shows a great slope, the state was found in a energy gap of approximately 0.54 eV. As we found the state is an hybridization of the $s$, $p_z$ atomic orbitals.

In the energy gap at $\bar{Y}$ point, we found two SS showing a parabolic shape. The lower state ($E_{S_6}$) is located at 1.46 eV. Our wavefunction for the $E_{S_6}$ state has the $p_y$ symmetry. This SS was found experimentally in Refs. [14, 19, 20], and theoretically in Refs. [13, 16]. The upper state ($E_{S_7}$) is located at 3.1 eV, and the state has the symmetries $s$, $p_z$. Experimentally this state was reported in Refs. [14, 18, 19], and theoretically in Ref. [16]. The energy difference found between our calculation and the reported values can be seen in Table IV.
TABLE IV: Calculated energy values for SS on the Ag(110) surface. The first column is the found SS, the second column list the $k$-point where the SS was found, the third column shows the experimental energy reported for the related state, the fourth list the theoretical energy value reported in the literature for the SS, the next column shows our calculated energy value for the found SS, finally the last column shows the symmetry of atomic orbitals that form the SS, according to our calculation. The $k$–vector are given in units of $[\frac{\pi}{a}]$, while the energies are in eV.

| surface state | $\vec{k}$ | $E_{\text{exp}}$ | $E_{\text{theo}}$ | $E_{\text{our}}$ | $SFO_{\text{our}}$ |
|---------------|-----------|------------------|-------------------|-----------------|------------------|
| $E_{\text{s}1}$ | $(\sqrt{2},0)$ | – | 4.18[16] | – | – |
| | | | 4.21[13] | 2.89 | $p_x$ |
| | | | | 2.04[19] | |
| $E_{\text{s}2}$ | $(\sqrt{2},0)$ | 4.86[14] | 5.26[19] | 6.16 | $s,p_z$ |
| $E_{\text{s}3}$ | $(\sqrt{2},0.4)$ | – | 8.06[19] | 9.22 | $p_y,z$ |
| $E_{\text{s}4}$ | $(\sqrt{2},1)$ | – | – | 6.43 | $s,p_z$ |
| $E_{\text{s}6}$ | (0,1) | –0.10[20] | 1.15[13] | 1.46 | $p_y$ |
| | | | 0.10[19] | – | – |
| | | | | 1.50[14] | 1.28[16] | 3.10 | $s,p_z$ |
| $E_{\text{s}7}$ | (0,1) | 1.65[18] | 1.95[19] | |

In the VB region we found four RS, and according to our calculations the states are: 1) The RS Er$_1$ is located at $\bar{\Gamma}$ at -5.12 eV, and its wavefunction has the full symmetry of the $d$ atomic orbitals. From the theoretical point of view, the state was reported in Ref. [16].

2) The RS Er$_2$ is located at $\bar{\Gamma}$ at -4.17 eV, and its wavefunction has also the full symmetry of the $d$ atomic orbitals. The state was calculated in Ref. [16].

3) The RS Er$_3$ is located at -3.40 at the $\bar{S}$ point, and its wavefunction has the symmetry of the $d_{x^2-y^2}$ atomic orbitals. Theoretically the state was reported in Ref. [16].

4) The RS Er$_4$ is found at -3.50 eV at $\bar{Y}$ point, and its wavefunction is an hybridization of the $d_{xy}$, $d_{xz}$ atomic orbitals.

Then, in the CB we found the RS Er$_5$, the state is located at 8.20 eV in the $\bar{S}$ point, and it wavefunction has the $p_y$ symmetry. The state was calculated in Ref. [16].
TABLE V: Calculated energy values for the RS of the Ag(110) surface. The first column shows the labeled resonance state, the second one shows the wavevector of the state in units of $[\pi/\sqrt{a}]$, the next column shows the related energy in eV, finally the last column shows the wave symmetry found for the different states.

| $E_r$ | $\vec{k}$ | $E_{\text{theo}}$ | $E_{\text{our}}$ | SFO$_{\text{our}}$ |
|------|-----------|----------------|----------------|------------------|
| Er$_1$ (0,0) | -4.74$^{16}$ | -5.12 | $d$ |
| Er$_2$ (0,0) | -3.76$^{16}$ | -4.17 | $d$ |
| Er$_3$ ($\sqrt{2}$,0) | -3.48$^{16}$ | -3.40 | $d_{x^2-y^2}$ |
| Er$_4$ (0,1) | -3.48$^{16}$ | -3.50 | $d_{xy,xx}$ |
| Er$_5$ ($\sqrt{2}$,0) | 7.52$^{19}$ | 8.20 | $p_y$ |
| Er$_6$ ($\sqrt{2}$/2,0) | 6.77$^{19}$ | 6.16 | $s,p_x$ |
| Er$_7$ (0,0) | -5.46 $d_{yz,x^2-y^2}$ |
| Er$_8$ (0,0) | 7.31 | $p_z$ |

The RS Er$_6$ is located at $\bar{\Gamma}$ at -5.46, and its wavefunction has the hybridization of the $s$, $p_x$ atomic orbitals. This state was also calculated in Ref. [16].

The RS Er$_8$ is located at $\bar{\Gamma}$ at 7.31 eV, and has the symmetry of the $p_z$ atomic orbitals.

As we found our calculated SS and RS for Ag(110) Es$_1$, Es$_2$, Es$_3$, Es$_6$, Es$_7$, Er$_1$, Er$_2$, ..., Er$_6$, have been reported previously in the literature, and in the usual precision of the method, show good agreement with them, as we can see in Tables IV and V. The new states found in this work are Es$_5$, Es$_8$, Es$_9$, Es$_{10}$, Es$_{10}$, Er$_7$ y Er$_8$.

D. Ag(111)

1. Projected bulk band structure, surface states, and resonance states

In an early calculation Ho et al. [21] by using the ab initio pseudopotential method, reported the bulk band structure, SS and RS for Ag(111). They predicted a SS just above the Fermi level in the $\Gamma$ point. Then in a photoemission measurement Kevan and Gaylord [22] corroborated the existence of this state at $\Gamma$ and present a discussion of it (see Fig. 5 in Ref. [22]).
Figure 2(c) shows our calculated projected bulk band structure for Ag(111). There we identify four SS labeled $E_{S2}$, $E_{S3}$, $E_{S8}$, and $E_{S9}$, and five RS labeled $E_{R1}$, ..., $E_{R5}$. In general, from the figure we observe that the calculated projected bulk bands structure are in agreement with that reported in Ref. [21]. The characteristics for the different found SS and RS are shown in Tables VI and VII.

2. Detailed discussion of the found SS and RS

The SS $E_{S2}$ is located in the lower gap at $-6.08$ eV at $\bar{\Gamma}$. The state shows a parabolic shape and its wavefunction is the hybridization of the $s, d_{3z^2-r^2}$ atomic orbitals.

Our found SS $E_{S3}$ was calculated at $2.28$ eV at $\bar{\Gamma}$, showing an important dispersion, its wavefunction has the symmetry of the $s, p_z$ atomic orbitals. From the experimental point of view a similar SS was reported by Altmann et al. [14] and Reihl et al. [23] as an unoccupied state, while Kevan and Gaylord et al. [22] reported the state as an occupied state. Theoretically in Ref. [21] the state was identified as an occupied state.

There are a couple of SS $E_{S8}$ and $E_{S9}$ located in the upper gap at $\bar{K}$. $E_{S8}$ was found at $6.63$ eV and its wavefunction has the symmetry of the $p_x, p_y$ atomic orbitals. $E_{S9}$ was calculated at $6.97$ eV, and its wavefunction has the symmetry of the $s, p_z$ atomic orbitals.

The RS $E_{R1}$ was calculated at $-6.42$ eV at $\bar{\Gamma}$, and we found that the state has the symmetry of the $d_{3z^2-r^2}$ atomic orbitals. Although there is no experimental evidence for this RS, theoretically the state was predicted in Ref. [21] (see Table VII for energy comparison).

In the energy bulk bands above the lower gap at $\bar{\Gamma}$, we found the state $E_{R2}$ at $-5.04$ eV, the calculated wavefunction for this RS was the hybridization of the $d_{xy,x^2-y^2}$ atomic orbitals. The state was reported in Ref. [21].

The state $E_{R3}$ was calculated at $-6.23$ eV at $\bar{M}$ point, and has the character of the $d$ orbitals. Theoretically, this state was predicted in Ref. [21].

The state $E_{R4}$ was calculated at $-3.82$ eV at $\bar{M}$ point, and its wavefunction has the symmetry of the $d_{xy,yz,zx,x^2-y^2}$ atomic orbitals. Theoretically, the state was reported in Ref. [21].

The state $E_{R5}$ was calculated in the lower border of the upper gap located in the $\bar{M}$ point. The state was located at $2.08$ eV, and has the symmetry of the $s, p_x, p_y$ atomic orbitals.

The states $E_{S3}$, $E_{R1}$, $E_{R2}$, $E_{R3}$ y $E_{R4}$ have been reported previously, and we found that our
calculations agree with the reported values, with the exception of the energy values for $E_{S3}$. The new states found in this work are $E_{S2}$, and $E_{r5}$.

**TABLE VI:** Surface states for the Ag(111). The first column is the found SS, the second column list the $k$-point where the SS was found, the third column shows the experimental energy reported for the related state, the fourth list the theoretical energy value reported in the literature for the SS, the next column shows our calculated energy value for the found SS, finally the last column shows the symmetry of atomic orbitals that form the SS, according to our calculation.

| $E_S$   | $\vec{k}$ | $E_{exp}$ | $E_{theo}$ | $E_{our}$ | SFO$_{our}$ |
|---------|-----------|-----------|------------|-----------|-------------|
| $E_{S2}$ (0,0) | 0.00[14] | -6.08 | $s, d_{3z^2-r^2}$ |
| $E_{S3}$ (0,0) | 0.33[23] | -0.31[22] | 2.28 | $s, p_z$ |
| $E_{S8}$ ($\frac{4}{3}\sqrt{2}, 0$) | -0.12[22] | 6.63 | $p_{x,y}$ |
| $E_{S9}$ ($\frac{4}{3}\sqrt{2}, 0$) | 6.97 | $s, p_z$ |

**TABLE VII:** Resonant states found for Ag(111) surface. The first column shows the labeled resonance state, the second one shows the wavevector of the state in units of $\left[\frac{\pi}{a}\right]$, the next column shows the related energy in eV, finally the last column shows the wave symmetry found for the different states.

| $E_r$ | $\vec{k}$ | $E_{teórico}$ | $E_{our}$ | SFO$_{our}$ |
|-------|-----------|------------|----------|-------------|
| $E_{r1}$ (0,0) | -6.26 [21] | -6.42 | $d_{3z^2-r^2}$ |
| $E_{r2}$ (0,0) | -5.04 [21] | -4.78 | $d_{xy,x^2-y^2}$ |
| $E_{r3}$ ($\sqrt{2}, \frac{\sqrt{6}}{3}$) | -6.26[21] | -6.01 | $d$ |
| $E_{r4}$ ($\sqrt{2}, \frac{\sqrt{6}}{3}$) | -3.82[21] | -3.36 | $d_{xy,yz,zz,x^2-y^2}$ |
| $E_{r5}$ ($\frac{4}{3}\sqrt{2}, 0$) | 2.08 | $s, p_x, p_y$ |
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[6] In a future work we will report a catalogue of SSs and RSs calculated using the ETB for several fcc and bcc transition and noble metals. (Preliminary work can be found in the H.J. Herrera–Suárez M.Sc. Thesis: http://www.fis.cinvestav.mx/~daniel/thesisend.pdf) (only in Spanish).

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