Adsorption of O and Cl on Tl/Si(111)—Suppressed spin polarization via bilayer formation

B. Pieczyrak[a,*], L. Jurczyszyn[a], M.W. Radny[b,c]

[a] *Institute of Experimental Physics, University of Wroclaw pl. Maxa Borna 9, 50-204, Wrocław, Poland*
[b] *Institute of Physics, Poznan University of Technology, ul. Piotrowo 3, 60-965, Poznan, Poland*
[c] *School of Mathematical and Physical Sciences, The University of Newcastle, Callaghan, 2308, Australia*

A B S T R A C T

Adsorption of O and Cl on Tl/Si(111) is studied using density functional theory. The surface of the Cl-Tl/Si(111) system was found to be metallic while that for O-Tl/Si(111), semiconducting. It is found, however, that the O/Tl and Cl/Tl interactions in Tl/Si(111) are very similar in nature and lead to the formation of the Tl-O and Tl-Cl bilayers weakly bonded to the Si(111)-1 × 1 substrate. The spin polarization of the Tl-induced gap states, originally present in Tl/Si(111), is also suppressed in both systems.

1. Introduction

In the last few years the adsorption systems that are composed of a semiconducting substrate and a monolayer of heavy elements with strong spin orbit interaction have attracted a lot of attention mainly due to their potential spintronic applications [1–19]. This is because of the formation of the interface electronic gap bands localized predominantly within the adlayer that are spin polarized. The bulk energy band gap of the semiconducting substrate prevents mixing of these spin polarized surface states with the unpolarized bulk states of the semiconductor. The spin splitting of the electronic bands at the interface is caused by the spin-orbit coupling and the electric potential gradient associated with the surface potential barrier, and is usually discussed within the Rashba-Bychkov model [20,21].

It was shown that in the systems that consist of the Si(111) and Ge (111) substrates covered by monolayers of Pb or Tl, the spin polarized 2D electron gas localized within the adlayer is decoupled from the substrate. It was also shown that the spin polarization of this 2D electronic gas is induced by the in-plane and out-of-plane bonding structure which modifies the in-plane symmetry of the charge distribution within the adlayer. This suppresses or enhances the surface spin polarization, as it takes place for the adsorption system with T1 and T4 geometry, respectively [18,19].

In this work we focus on the oxygen and chlorine interaction with the Tl/Si(111) system. We show that the O-Tl and Cl-Tl interactions lead to the formation of the Tl-O and Tl-Cl bilayers weakly bonded to the Si substrate with the corresponding surface band structures containing the gap states with the spin polarization completely suppressed. Our data also shows that while the interaction of Cl and O with the Tl adatoms are similar in nature the observed differences in the Tl-Si(111) bonded structure results from the structural differences within the formed O-Tl and Cl-Tl bilayers.

2. Methodology

The density functional theory (DFT) calculations with the spin-orbit interaction (SOC) were performed using Vienna Ab-initio Simulation Package (VASP) [22–25]. The Tl/Si(111)-1 × 1 system was modeled by the six layer slab of Si atoms with one side covered by a 1 × 1 Tl layer and the opposite side saturated by H atoms. The adsorption of oxygen/ chlorine atoms was investigated for the 1 × 1 Cl/O monolayer located at the T4, H3 and T1 adsorption sites above the Tl adlayer. In the total energy calculations the five topmost silicon layers, Tl atomic layer and oxygen/chlorine adlayer were allowed to relax. The relaxation process, using the conjugate gradient method and the Davison-Block algorithm [26], was carried out until the forces acting at the relaxed atoms were less than 0.01 eV/A. The PAW potentials [27,28] were adopted to describe the electron-ion interaction and the exchange-correlations

---

The presence of the unsaturated dangling bonds on the Si(111)1 × 1 substrate have been calculated within the 1 × 1 unit cell and any possible reconstruction of the Si(111) substrate has not been investigated.

* Corresponding author.
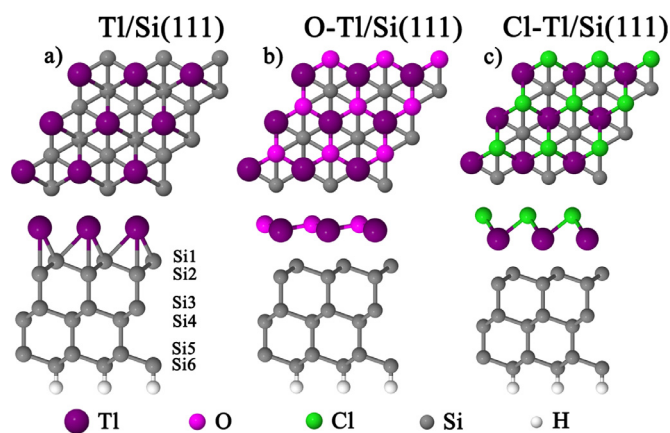 *E-mail address:* meghan@ifd.uni.wroc.pl (B. Pieczyrak).

Fig. 1. Schematics of the most stable atomic configurations of the (a) Tl/Si (111) – T4, (b) O-Tl/Si(111) – H3 and (c) Cl-Tl/Si(111) – H3 adsorption systems. Top and side views are shown.

contributions were treated within the GGA-PBE approach [29,30].

3. Results and discussion

Our initial total energy calculations for the Tl/Si(111) system have confirmed that the Si(111)-1 × 1 surface with a 1 × 1 monolayer of Tl atoms located at the T4 sites is the most energetically favorable (see Fig. 1a). This structure is by 0.09 eV and 0.36 eV lower in energy than the 1 × 1 Tl monolayer located on Si(111)1 × 1 at H3 and T1, respectively. These agree with other published data [11]. The binding energy of the Tl adatom to the Si(111)-1 × 1 substrate in the most stable configuration is calculated to be 1.2 eV.

The electronic surface band structure calculated for the most stable T4 configuration are presented in Fig. 2a and b. They are also observed to reproduce previous results [11]. The relativistic (SOC) surface band structure shown in Fig. 2a is semiconducting. The empty, spin split surface bands located within the Si(111) bulk band gap above the Fermi level (S1 and S2) are formed predominantly by the Tl p_x-p_y states. These states are decoupled from the substrate bulk states and are not involved in the Tl-Si interaction, as illustrated by the corresponding partial charge distribution presented in Fig. 3a. This is why the spin-splitting in bands S1 and S2 does not originate from the electric gradient of the surface potential barrier as described by the classical Rashba-Bychkov model. The reason is that the two dimensional electronic gas (2DEG), described by states in bands S1 and S2, is isolated from the interaction with the silicon substrate and as such it is not affected by the substrate-induced structural asymmetry. It was shown earlier[18] that in the Pb/Si(111) system, that has very similar electronic properties to Tl/ Si (111), the spin polarization of the states associated with the 2DEG decoupled from a substrate (bands S1 and S2 in Fig. 2a) can be induced by the in-plane bonding structure within the (Pb or Tl) adlayer, i.e., the bonding structure can break the in-plane symmetry of the charge distribution within the2DEG and enhance the adatom spin-orbit coupling, as illustrated in Fig. 2a for the Tl/Si(111) system. This is the case for systems with the T4 adsorption geometry (considered in Fig. 2a). A different behavior, however, can be observed in the adsorption systems with the T1 geometry (not shown in Fig. 2) - the unbroken, in this case, in-plane symmetry of the 2DEG charge distribution suppresses the spin polarization of the gas states. Interestingly, both scenarios are present in real systems since in Tl/Si(111) the T4 geometry (considered in Fig. 2a) is most energetically favorable, while in Pb/Si(111) the lowest energy configuration is associated with the T1 structure.

The occupied surface bands (S3 and S4) are composed of the Tl p_x-p_y states and the Si p_z states, and as such these states are directly involved in the Tl-Si bond formation. The covalent type of this interaction is visible in the partial charge distribution shown in Fig. 3b. The lack of

spin polarization in these bands (compare SOC and non-SOC band structures in Fig. 2a and b, respectively) results from the Tl-Si bonding.

The data presented for Tl/Si(111) are very similar to that obtained for the Pb/Si(111) system with the spin split bands (S1 and S2 in Fig. 2a) shifted toward lower energies due to different number of Pb valence electrons. As a consequence the spin polarized bands in Pb/Si (111) cross the Fermi level and are partly occupied [31]. This is contrary to the Tl/Si(111) system (see Fig. 2).

3.1. Adsorption of oxygen

The adsorption of O on the most stable Tl/Si(111) structure has been examined for the 1 × 1 O-adlayer located at the T4, H3 and T1 sites of the Tl/Si(111) substrate. The H3 configuration has been found to be the most energetically favorable (see Fig. 1b) with the T4 and T1 configurations being higher in energy by 0.19 eV and 2.25 eV, respectively. The structural parameters calculated for the most stable O/ Tl/Si(111) structure are shown in Table 1. One observes that upon adsorption the O-Tl bond has the bond length of 2.27 Å, and is associated with the increase of the Tl-Si bond length from 3.20 Å to 3.37 Å. Moreover, the atoms of the O monolayer are almost incorporated into the Tl monolayer as the vertical separating between the layers is just 0.43 Å (see Fig. 1b). The binding energy of the Tl-O bilayer to the Si (111)-1 × 1 substrate is calculated to be 0.5 eV. This is much lower than the adsorption energy of 1.2 eV calculated for the Tl monolayer in the Tl/Si(111) adsorption system.

The weak bonding between the O-Tl bilayer and the Si substrate is also reflected in the calculated band structures presented in Fig. 2, where Fig. 2c shows the SOC band structure of the energetically most stable O-Tl-Si(111) configuration, Fig. 2e shows the SOC band structure of the isolated Tl-O bilayer with the O and Tl positions extracted from the relaxed O-Tl-Si(111) system (see Fig. 1b), Fig. 2d presents the band structure of Si(111)-1 × 1 with the Tl-O bilayer separated by 8.8 Å (non-SOC) is presented, and Fig. 2f shows the electronic structure of clean, unreconstructed Si(111)-1 × 1.

As expected, the band structure of the O-Tl bilayer separated from clean Si(111) (Fig. 2d) is a simple combination of the bands of Fig. 2e (isolated Tl-O) and those of Fig. 2f (clean Si(111)-1 × 1). We also observe that the band structure of Fig. 2d is very well reproduced in the band structure of the O-Tl/Si(111) adsorption system shown in Fig. 2c; the only difference between these band structures are seen at the two k-points where the bands cross in Fig. 2d, while in Fig. 2c the crossing is avoided. These similarities between the band structures of Figs. 2c and d demonstrate that the formation of the O-Tl bilayer weakens the Tl_Si bonding and leads to a reduced interaction between the Si(111)-1 × 1 substrate and the O-Tl bilayer.

The features identified in the electronic band structure of O/Tl/Si (111) are consequences of the bonding within the O-Tl bilayer. We observe that while in the Tl/Si(111) system the Tl s-orbitals are inactive, in the presence of oxygen they form a strong bond with the O p_x-p_y states. This is evidenced by the data in Table 2 and illustrated by the corresponding partial charge distribution shown in Fig. 4a. The band that represents the bonding character of these states lies 6.4 eV below the Fermi level and is not shown in Fig. 2. However, the antibonding character of the Tl(s) –O(p_x-p_y) bond can be seen in the states that form bands S5* and S5 in Fig. 2e and c, respectively. This is illustrated by the probability density distribution calculated for band S5 at the K point shown in Fig. 4b (see also Table 2).

The O-Tl interaction also destroys the Tl-Si bonds, (S3 and S4 in Fig. 2a), and leads to the formation of the unsaturated Si dangling bonds (p_z) characteristic for the clean, unreconstructed Si(111)-1 × 1 substrate[†]. These states on Si(111)-1 × 1 form a non-dispersive, metallic gap band (blue curve in Fig. 2f) that in the non-interacting O-Tl/Si (111) system (Fig. 2d) crosses the antibonding Tl-O band (S5* in Fig. 2e). In the band structure of the O-Tl-Si(111) adsorption system (Fig. 2c) the crossings are avoided resulting in the semiconducting band
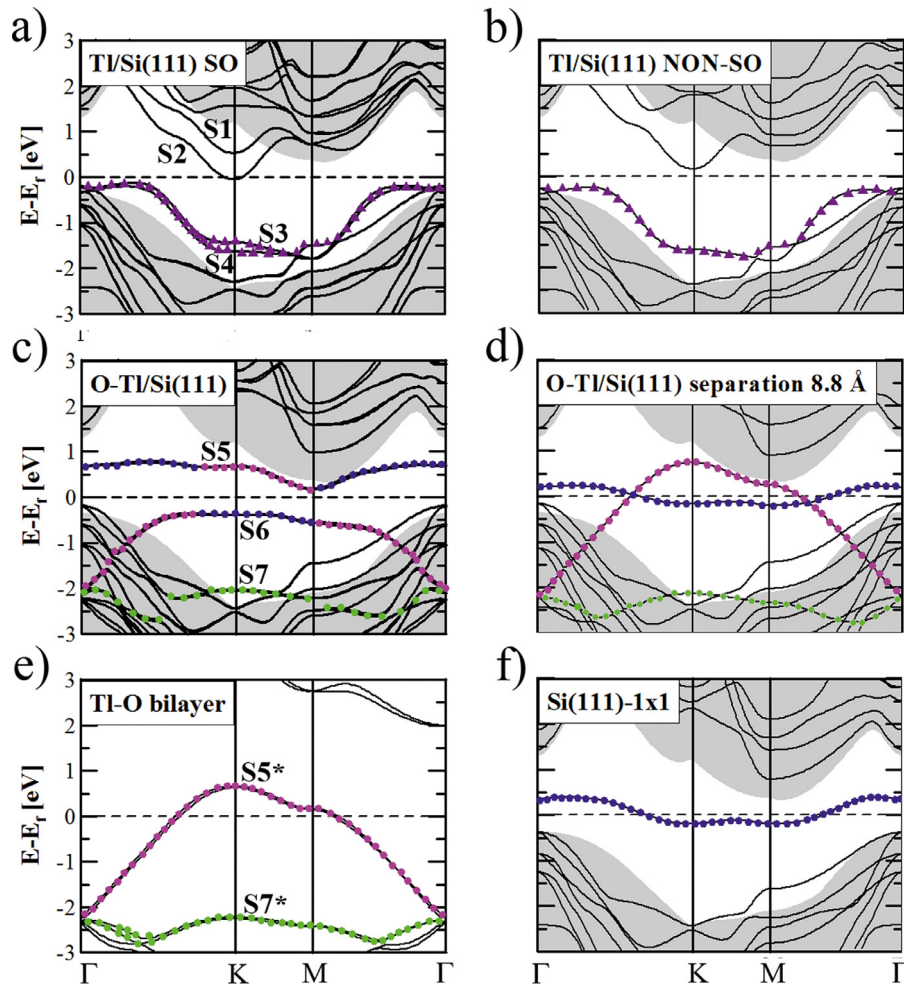
Fig. 2. Surface electronic band structures of (a) Tl/Si(111) in configuration T4 with SOC and (b) without SO; (c) O-Tl/Si(111) (with SOC); (d) Tl-O bilayer separated by 8.8 Å (non-SOC); (e) isolated Tl-O bilayer (with SOC), and (f) Si(111)-1 × 1 (non-SOC). The shaded area represents the bulk Si band structure projected on the [111] direction. The Fermi energy is at 0.0 eV.
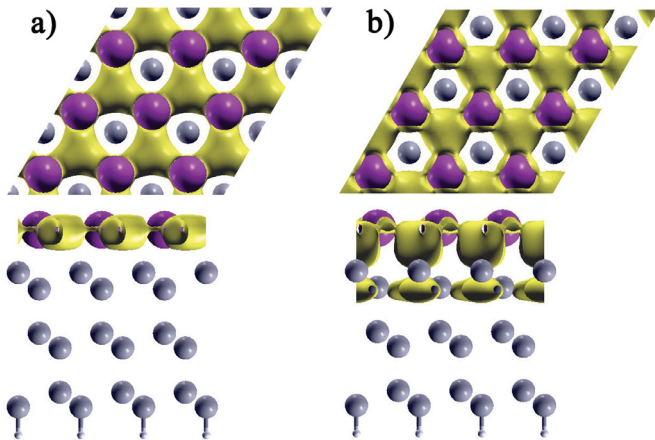

Fig. 3. Top and side views of the SO partial probability and charge distributions calculated at point K of the electronic states of band (a) S1 and (b) S4 from Fig. 2a. Isosurface value: 0.00015 e/ Å^3 and 0.0001 e/ Å^3 for (a) and (b), respectively.

structure.

3.2. Adsorption of chlorine

The configuration with the Cl adatoms located at the H3 adsorption

Table 1
Calculated atomic distances and interlayer spacings, Δz, (in Å) within the Tl/Si(111), O-Tl/Si(111) and Cl-Tl/Si(111) adsorption systems. The enumeration of Si atoms is shown in Fig. 1.

Atom	Distance			Δz		
	Tl/Si (111)	O-Tl/Si (111)	Cl-Tl/Si (111)	Tl/Si (111)	O-Tl/Si (111)	Cl-Tl/Si (111)
O-Tl	–	2.27	–	–	0.43	–
Cl-Tl	–	–	2.85	–	–	1.77
Tl-Si1	3.20	3.37	3.44	2.30	2.53	2.61
Si1-Si2	2.40	2.37	2.36	0.87	0.79	0.78
Si2-Si3	2.37	2.38	2.38	2.37	2.38	2.38

site of the Tl/Si(111) system was found to be the most energetically favorable (see Fig. 1c). This is similar to the adsorption of O on Tl/Si(111). The structural data in Table 1 shows that upon adsorption the Cl-Tl bond is formed with the bond length of 2.85 Å accompanied by the increase of the Tl-Si bond length from 3.20 Å to 3.44 Å. As a result the distance between the Tl monolayer and the Si substrate increases from 2.30 Å to 2.61 Å, with the Tl and Cl layers separated by only 1.77 Å. The latter value is considerably larger than the separation between O and Tl layers in O-Tl/Si(111) system (0.43 Å). However, these structural changes result in a calculated binding energy of the Cl-Tl bilayer to the Si(111) substrate of just 0.3 eV, which is slightly lower than the binding energies of the O-Tl bilayer (0.5 eV) in O-Tl/Si(111).

The origin of the weak bonding between the Cl-Tl bilayer and the Si

Table 2

The s, p_z, p_{xy} projected wave function character of the bands calculated at the K point for SOC band structures of O/Tl/Si(111) (Fig. 2c) and Cl/Tl/Si(111) (Fig. 5b). The corresponding data for the bands S3 and S4 of the Tl/Si(111) system (Fig2) are also shown (top panel). Denotations of bands are the same as in Figs. 2 and 5. Description "band of bonding states" denotes the electronic band composed of the Tl s and O/Cl p_{xy} states located 6.4 eV and 5.0 eV below the Fermi level (for O/Tl/Si(111) and O/Tl/Si(111), respectively). The corresponding data obtained for isolated O-Tl and Cl-Tl bilayers are also shown.

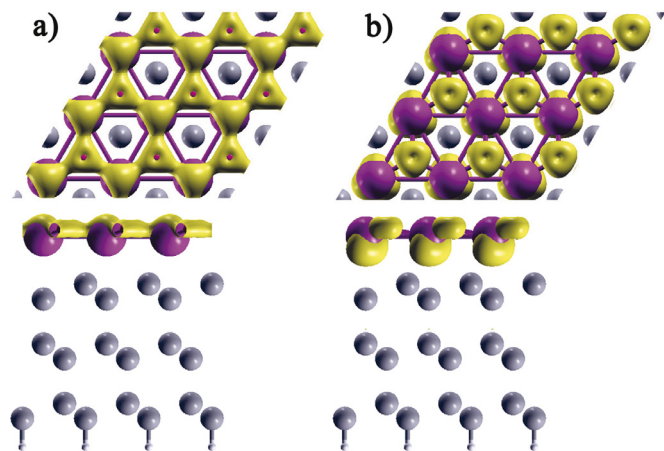| System	Atom	S	p_z	p_x p_y
Tl/Si(111) band S3	Tl	–	–	0.076
	Si	–	0.159	–
Tl/Si(111) band S4	Tl	–	–	0.104
	Si	–	0.140	–
O/Tl/Si(111) band S5	O	–	–	0.312
	Tl	0.188	0.052	–
	Si	–	–	–
O/Tl/Si(111) band S6	O	–	–	0.060
	Tl	–	–	–
	Si	0.034	0.187	–
O/Tl/Si(111) band of bonding states	O	–	–	0.186
	Tl	0.296	0.003	–
	Si	–	–	0.010
O-Tl bilayer band S5*	O	–	–	0.390
	Tl	0.240	0.065	–
O-Tl bilayer band of bonding states	O	–	–	0.250
	Tl	0.439	–	–
Cl/Tl/Si(111) band S9	Cl	–	–	0.060
	Tl	–	–	0.026
	Si	0.019	0.170	–
Cl/Tl/Si(111) band S10	Cl	–	–	0.262
	Tl	0.233	0.020	–
	Si	–	–	0.012
Cl/Tl/Si(111) band of bonding states	Cl	–	–	0.184
	Tl	0.396	0.005	–
	Si	–	–	–
Cl-Tl bilayer band S10*	Cl	–	–	0.366
	Tl	0.264	0.042	–
Cl-Tl bilayer band of bonding states	Cl	–	–	0.196
	Tl	0.430	0.006	–

Fig. 4. (a) Partial charge distribution illustrating the bonding between the Tl s and O p_x-p_y states. The corresponding band is located 6.4 eV below the Fermi level. (b) Partial probability and charge distributions for the states that compose band S5 in Fig. 2c. All distributions are calculated with SOC at point K with the isosurface value of 0.0002 e/ Å^3.

substrate can be deduced from both the atomic configuration of the Cl-Tl/Si(111) system and the corresponding electronic band structure shown in Fig. 5. In the Cl-Tl/Si(111) system the Cl atoms in the Cl-Tl bilayer are located considerably above Tl atoms. This is because the ionic radius of chlorine adatom is significantly greater than that for oxygen and therefore chlorine atoms are not able to penetrate Tl-1 × 1
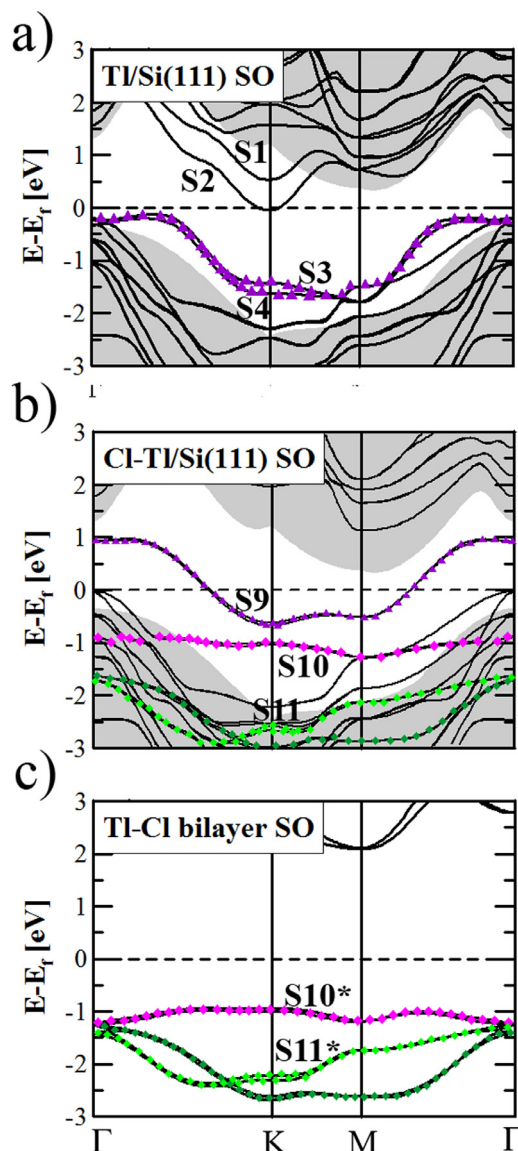

Fig. 5. SOC electronic band structures of (a) Tl/Si(111), (a) Cl-Tl/Si(111), and (c) the isolated Tl-Cl bilayer. The shaded area represents the bulk Si band structure projected on the [111] direction. The Fermi energy is at 0.0 eV.

layer like oxygen in O-Tl/Si(111) system. In this configuration the Tl-Si bonds in Cl-Tl/Si(111) are significantly weakened by the adsorption of Cl, but not destroyed. Figs. 5a and b shows the SOC band structures of Tl/Si(111) and the energetically most stable Cl-Tl-Si(111) configuration, respectively. We observe that the shape of the metallic gap band (S9) in the electronic structure of Cl-Tl/Si(111) is identical to the shape of the occupied gap band (S3/S4) in the structure for the Tl/Si(111) system. The states within bands S4/S3 describe the bonding between the Tl (p_x-p_y) and Si p_z (dangling bond) states. The presence of the metallic band (S9) in the band structure of Fig. 5b suggests, therefore, that the interaction of Cl with Tl/Si(111), while not destroying the Tl-Si bonding structure, reduces its strength. This is due to the transition of the state representing the Tl-Si bond from being completely occupied for Tl/Si(111) to become metallic for Cl-Tl/Si(111). This metallic gap state remains spin unpolarized, similarly to the Tl/Si(111) system.

We have found that in the Cl-Tl-Si(111) system the Tl s states are involved in the formation of the bond with the Cl p_x-p_y states (see Table 2). The band that represents the bonding combination of these states is located 5.0 eV below the Fermi level (not shown in Fig. 5b) - the corresponding spatial charge distribution is presented in Fig. 6a.
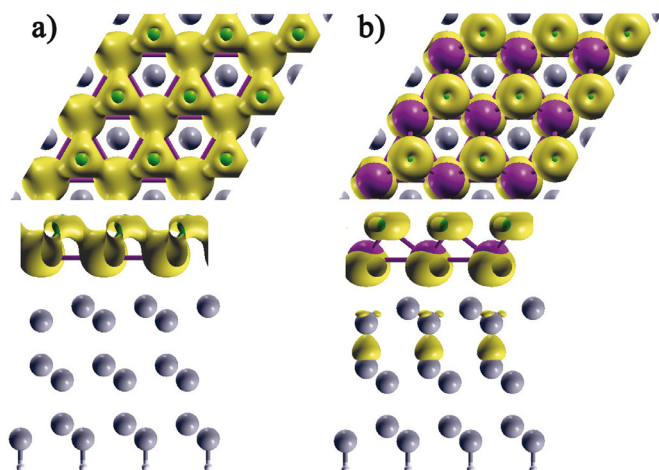
Fig. 6. (a) Partial charge distribution illustrating the bonding between the Tl and the p_x-p_y states of Cl atoms. The band associated with these states is located 5 eV below the Fermi level. (b) Partial charge distributions for the electronic states from the band S10 in Fig. 2c. All charge distributions are calculated with SOC at point K. Isosurface value: 0.00015 e/ Å^3 for (a) and 0.0001 e/ Å^3 for (b).

This indicates that the Cl p_x-p_y states are mixed with the Tl s states and that these states are responsible for the Tl-Cl bilayer bonding structure. The corresponding antibonding combination of these states can be seen in band S10 of Fig. 6b. Comparison with Fig. 5c, where the band structure of the isolated Cl-Tl bilayer is presented, clearly shows that band S10 in Fig. 5b originates from band S10* of the isolated Cl-Tl bilayer.

Similarly band S11 in Fig. 5a originates from band S11* in the band structure of the isolated Cl-Tl bilayer (Fig. 5c). The obtained results shows, that around point K bands S11 and S11* are composed entirely of the p_z states of the Cl atoms.

4. Conclusions and summary

The effect of adsorption of oxygen and chlorine monolayers on Tl/Si (111) was investigated with the focus on the structural, and electronic and spin properties of the system. We found that in both cases the O/Tl and Cl/Tl interactions lead to the formation of the O-Tl and Cl-Tl bilayers weakly bonded to the Si(111) substrate. The bonding within the O-Tl and Cl-Tl bilayers was shown to be very similar in nature. In both systems the Tl s states were shown to involved in the formation of the bond with the O and/or Cl p_x-p_y states. The bands representing the bonding combination of these states are located 6.4 eV/5.0 eV below the Fermi level while the corresponding bands composed of antibonding combination states appear within the energy gap of the O-Tl/Si (111) and Cl-Tl/Si(111) systems. We found that the O-Tl and Cl-Tl interactions lead to almost complete suppression of the spin polarization originally present in the gap states of the Tl/Si(111) system.

We have also identified some differences between the studied systems. In the O-Tl bilayer the oxygen atoms were found to be almost incorporated into the Tl-1 × 1 layer with the Tl-Si bonds broken and the dangling bonds of the Si(111) substrate unsaturated. Consequently, the O-Tl/Si(111) surface band structure shows the presence of the gap states originating from the dangling bonds of the Si(111)-1 × 1 substrate and the electronic structure of the O-Tl/Si(111) system was found to be semiconducting. By contrast, in the Cl-Tl/Si(111) system the Cl atoms in the Cl-Tl bilayer were found to be located considerably above the Tl atoms. In this configuration the Tl-Si bonds in Cl-Tl/Si(111) are significantly weakened by the adsorption of Cl, but not destroyed, as it is the case for the O-Tl/Si(111) system. The Tl-Si bond is weakened in Cl-Tl/Si(111) mainly due to the fact that the corresponding band

structure is metallic. This is because the metallic gap band that crosses the Fermi level consists of the states involved in the bonding between Tl and the topmost Si atoms and as such is virtually the same as the occupied band in the band structure of the undisturbed Tl/Si(111) system.

CRediT authorship contribution statement

B. Pieczyrak: Software, Formal analysis, Investigation, Writing - original draft, Writing - review & editing, Visualization. **L. Jurczyszyn:** Investigation, Writing - original draft, Writing - review & editing. **M.W. Radny:** Conceptualization, Investigation, Writing - review & editing.

Declaration of Competing Interest

None.

Acknowledgments

References

[1] A. Manchon, H.C. Koo, J. Nitta, S.M. Frolov, R.A. Duine, Nat. Mat. 14 (2015) 871.
[2] S.D. Stolwijk, A.B. Schmidt, N. Donath, K. Sakamoto, P. Krüger, Phys. Rev. Lett. 111 (2013) 176402.
[3] K. Sakamoto, T. Oda, A. Kimura, K. Miyamoto, M. Tsujikawa, A. Imai, N. Ueno, H. Namatame, M. Taniguchi, P.E.J. Eriksson, R.I.G. Uhrberg, Phys. Rev. Lett. 102 (2009) 096805.
[4] P.E.J. Eriksson, K. Sakamoto, R.I.G. Uhrberg, Phys. Rev. B 81 (2010) 205422.
[5] S. Y.Ohtsubo, H.O Hatta, T. Aruga, J. Phys.: Cond. Matt. 24 (2012) 092001.
[6] S. Hatta, T. Aruga, C. Kato, S. Takahashi, H. Okuyama, A. Harasawa, T. Okuda, T. Kinoshita, Phys. Rev. B 77 (2008) 245436.
[7] S. Hatta, C. Kato, N. Tsuboi, S. Takahasi, H. Okuyama, T. Aruga, A. Harasawa, T. Okuda, T. Kinoshita, Phys. Rev. B 76 (2007) 075427.
[8] K. Yaji, S. Hatta T. Aruga, H. Okuyama, Phys. Rev. B 86 (2012) 235317.
[9] K. Sakamoto, T.H. K.im, T. Kuzumaki, B. Müller, Y. Yamamoto, M. Ohtaka, J.R. Osiecki, K. Miyamoto, Y. Takeichi, A. Harasawa, S.D. Stolwijk, A.B. Schmidt, J. Fujii, R.I.G. Uhrberg, M. Donath, H.W. Yeom, T. Oda, Nat. Commun. 4 (2013) 2073.
[10] K. Yaji, Y. Ohtsubo, S. Hatta, Okuyama H, K. Miyamoto, T. Okuda, A. Kimura, H. Namatame, M. Taniguchi, T. Aruga, Nat. Commun. 17 (2010) 1.
[11] J. Ibañez-Azpiroz, A. Eiguren, A. Bergara, Phys. Rev. B 84 (2011) 125435.
[12] L. Petersen, P. Hedegard, Surf. Sci. 459 (2000) 49.
[13] Y.M. Koroteev, G. Bihlmayer, J.E. Gayone, E.V. Chulkov, S. Blügel, P.M. Echenique, P. Hofmann, Phys. Rev. Lett. 93 (2004) 046403.
[14] I. Gierz, T. Suzuki, E. Frantzeskakis, S. Pons, S. Ostanin, A. Ernst, J. Henk, M. Grioni, K. Kern, C.R. Ast, Phys. Rev. Lett. 103 (2009) 046803.
[15] C.R. Ast, J. Henk, A. Ernst, L. Moreschini, M.C. Falub, D. Pacilé, P. Bruno, K. Kern, M. Grioni, Phys. Rev. Lett. 98 (2007) 186807.
[16] T. Zhang, P. Cheng, W.-.J. Li, Y.-.J. Sun, G. Wang, X.-.G. Zhu, K. He, L. Wang, X. Ma, X. Chen, Y. Wang, Y. Liu, H.-.Q. Lin, J.-.F. Jia, Q.-.K. Xue, Nat. Phys. 6 (2010) 104.
[17] K. Sakamoto, H. Kakuta, K. Sugawara, K. Miyamoto, A. Kimura, T. Kuzumaki, N. Ueno, E. Annese, J. Fujii, A. Kodama, T. Shishidou, H. Namatame, M. Taniguchi, T. Sato, T. Takahashi, T. Oguchi, Phys. Rev. Lett 103 (2009) 156801.
[18] B. Pieczyrak, M. Szary, L. Jurczyszyn, M.W. Radny, Phys. Rev. B 93 (2016) 195318.
[19] M. Szary, B. Pieczyrak, L. Jurczyszyn, M.W. Radny, Appl. Surf. Sci. 466 (2019) 224.
[20] E.I. Rashba, Sov. Phys. Solid State 2 (1960) 1109.
[21] Y.A. Bychkov, E.I. Rashba, JETP Lett 39 (1984) 78.
[22] G. Kresse, J. Hafner, Phys. Rev. B 47 (1993) 558.
[23] G. Kresse, J. Hafner, Phys. Rev. B 49 (1994) 14251.
[24] G. Kresse, J. Furthmüller, Comput. Mat. Sci. 6 (1996) 15.
[25] G. Kresse, J. Furthmüller, Phys. Rev. B 54 (1996) 11169.
[26] E.R. Davison, Methods in Computational Molecular Physics, Plenum, New York, 1983.
[27] P.E. Blöchl, Phys. Rev. B 50 (1994) 17953.
[28] G. Kresse, D. Joubert, Phys. Rev. B 59 (1999) 1758.
[29] J.P. Perdew, K. Burke, M. Ernzerhof, Phys. Rev. Lett. 77 (1996) 3865.
[30] J.P. Perdew, K. Burke, M. Ernzerhof, Phys. Rev. Lett. 78 (1997) 1396.
[31] A. Araki, T. Nishijima, M. Tsujikawa, T. Oda, J. Phys. 200 (2010) 062001.