ELECTRONIC STRUCTURE OF THE INTERFACE OF GAAS(110)/SB(xL)

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INTRODUCTION

The electronic structure of the surface of GaAs covered with Sb was calculated by using the extended-Hückel theory. In order to get a parametrization of the one-particle Hamiltonian the known surface electronic structure of the system GaAs(110)-p(1x1)-Sb(1ML)[3,4] was interpolated. The knowledge of these parameters together with those being obtained from bulk Sb as well as bulk GaAs parametrizations allows to calculate the electronic structure of GaAs(hkl)/Sb(xL) for a presumed atomic geometry. The system GaAs(110)-p(1x1)-Sb(2L) is analysed, the surface atomic geometry being determined by a total-energy-minimization[5]. For a thicker overlayer the incommensurability of the bulk Sb and GaAs crystal structures has to be considered. It is treated by the use of averaged layer-coupling constants. Additionally the recursion procedure for the semi-infinite crystal[1,2] is extended to interfaces between two arbitrary bulk systems, so that interface states of the GaAs-Sb-interface can be analysed.

AVERAGED LAYER COUPLING CONSTANTS

In order to calculate the elements of the overlap matrix $\underline{S}$ belonging to the last layer in GaAs-structure and the first layer in Sb-structure it is a good approximation to confine the summation to the next neighbour term:

$$S_{q\beta mp\alpha l}(\vec{k}_{\|}) = \frac{1}{N_{\|}} \sum_{j=1}^{N_{\|}} \sum_{h\in \mathrm{NN}} \exp\left[i\,\vec{k}_{\|}\left(\vec{R}^{\|}_{ljp} - \vec{R}^{\|}_{mhq}\right)\right] \cdot$$
$$\cdot \langle \alpha, 0 \mid \beta, \mid \vec{R}^{\|}_{ljp} - \vec{R}^{\|}_{mhq} \mid \rangle$$

where $N_{\|}$ is the number of planar unit cells, jpl is the index for the l^{th} atom of the basis in the j^{th} unit cell of the p^{th} layer, $\langle\rangle$ denotes the overlap integral.

This sum cannot be simplified since all the unit cells are different because of the incommensurability. The directions of the vectors $(\vec{R}^{\|}_{ljp} - \vec{R}^{\|}_{mhq})$ are isotropically distributed and for all j (h) there exist indices i (k), such that $\mid (\vec{R}^{\|}_{ljp} - \vec{R}^{\|}_{mhq}) - (\vec{R}^{\|}_{lip} - \vec{R}^{\|}_{mkq}) \mid$ is arbitrarily small, i. e. the vectors constitute a dense set. These facts enable the transition from the summation to an integration, the introduction of plane polar coordinates and a further approximation of this integral by a sum:

$$S_{q\beta mp\alpha l}(\vec{k}_{\|}) = \aleph \frac{1}{M} \sum_{j=1}^{M} \mid \vec{r}_j \mid \exp\left(i\vec{k}_{\|}\vec{r}_j\right) \cdot$$
$$\cdot \langle \alpha, 0 \mid \beta, \mid \vec{r}_j{}^{\|} \mid \rangle\, \Delta r_j \Delta\phi_j$$

For our calculations we have chosen M = 100 integration points distributed on concentric circles, $\Delta\phi_j = \Delta\phi$ and $\Delta r_j = \Delta r$.

The additional factor $\aleph = A_{GaAs}/A_{Sb}$ considers the different sizes of the GaAs and Sb unit cells.

These averaged overlap matrix elements are referenced as averaged layer coupling constants. The interface is treated by a straightforward extension of the surface renormalization scheme.

RESULTS

Fig.1 shows the surface electronic structure of the GaAs(110)-p(1x1)-Sb(1ML) system in comparison with the GaAs(110)/ Sb(1L) system. Though this ideal configuration does not represent the well established physical picture of a one-overlayer reconstruction, it has been included for convenience. The bandstructure already shows the typical features of all those systems with ideal Sb(xL) (fig.5, fig.6, fig.7), namely a cumulation of p-type surface states in the fundamental gap distributed over the Sb-layers.

The next step is the analysis of systems with two layers of Sb on the (110)surface of GaAs. The atomic geometry has been determined by a total-energy minimization[5] on the assumptions, that the relaxation of the GaAs layers and the 1st Sb layer remains unchanged when the 2nd layer Sb is adsorbed, that the two-dimensional unit cell of the 2nd layer Sb is rectangular and has a two-point basis, and that the mirror-plane symmetry may be destroyed by a relaxation in x-direction. The following data represent the obtained differences from the positions in an ideal zincblende lattice:
$\Delta\vec{r}_1 = (-0.09555,\ -0.2454,\ 0.9872)$Å,
$\Delta\vec{r}_2 = (-0.0613,\ 0.4206,\ 1.2061)$Å. The relaxation of the 2nd layer Sb is very strong in comparison with the 1st layer (fig.8).

Fig.2 represents the resulting surface electronic structure which is rather different from that of the remaining two calculated overlayer systems, GaAs(110)/Sb(2L) (fig.6) and GaAs(110)-p(1x1)-Sb(1ML)/Sb(1L) (fig.5), containing ideal Sb layers. The crystal surface is expected to be metallic because there is a very dispersive state p_z-like in character crossing the Fermi level (0.84eV) several times. The hatched underground in fig.2 represents the projected band structure of bulk GaAs as well as of bulk Sb. It could be expected that the electronic bands lying in gaps of both projected structures will be observed at the GaAs-Sb interface in systems with more than two layers of Sb. Especially the variety of states in the GaAs stomach gap which is not covered by the projected Sb structure seems to fulfil this assumption.

To clear this point higher Sb-coverages were investigated. In contrast to the first guess the existence of interface states in the stomach gap could not be confirmed, however, they were found in the fundamental gap of GaAs, especially for the GaAs(110)/Sb(3L) and the GaAs(110)/Sb systems (fig.3, fig.4), being ($p_x p_y p_z$)-like in character. Both systems show interface states localized in the last GaAs-layer. Additionally only the GaAs(110)-Sb system has interface states localized in the first Sb-layer lying near the edge of the projected Sb bulk band structure.

- Interface states are found in systems with more than two Sb-layers.
- A coverage of Sb(3L) is not sufficient to separate the Sb surface from its interface.
- The interface states of sytems with several Sb-layers should be detectable in photoemission experiments.

References

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Denotation

" / " denotes the separation of the GaAs-structure from the ideal Sb-structure.

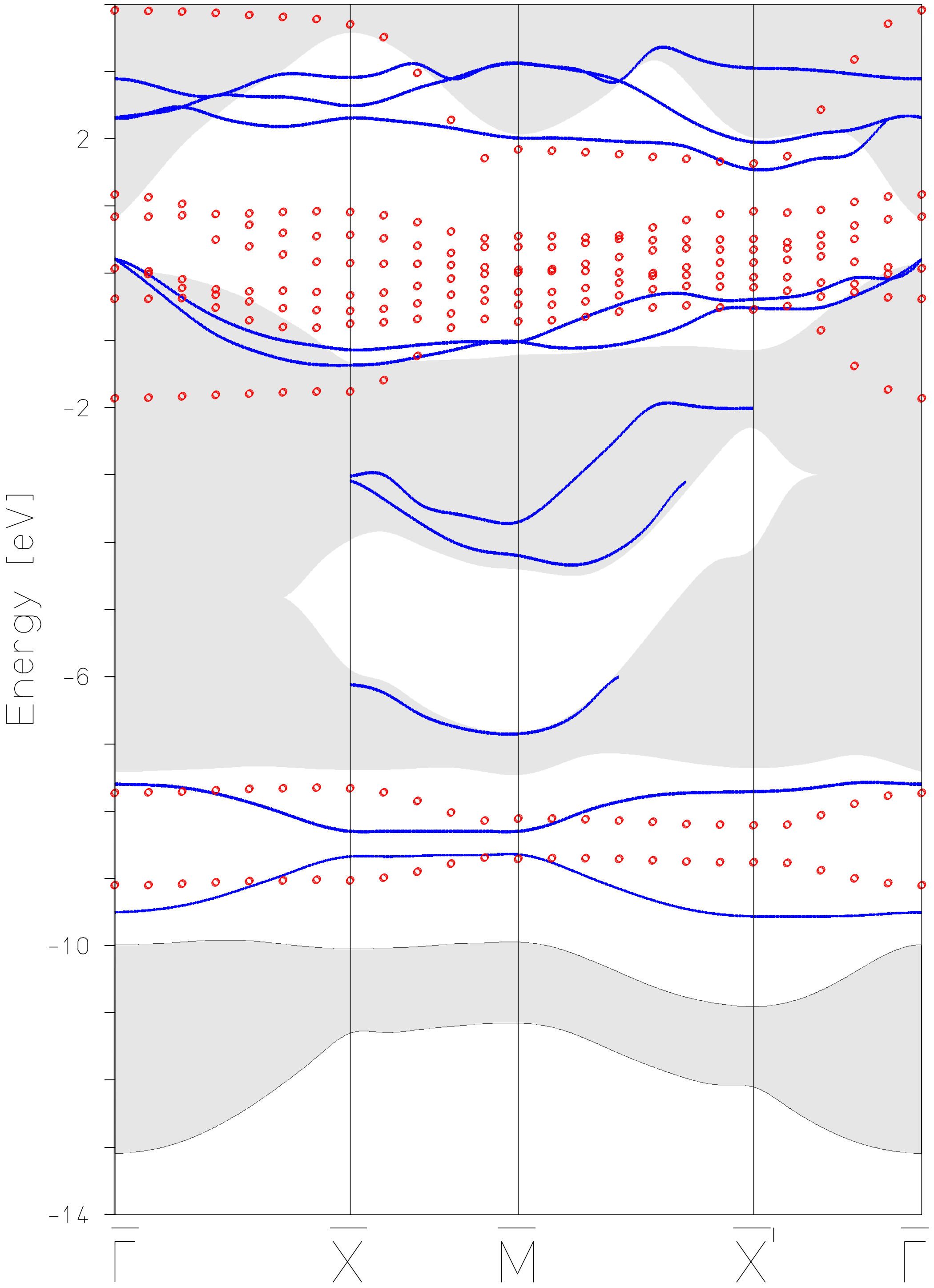

Figure 1: Surface electronic structure of the systems GaAs(110)-p(1x1)-Sb(1ML) (blue lines) and GaAs(110)/Sb(1L) (red circles).

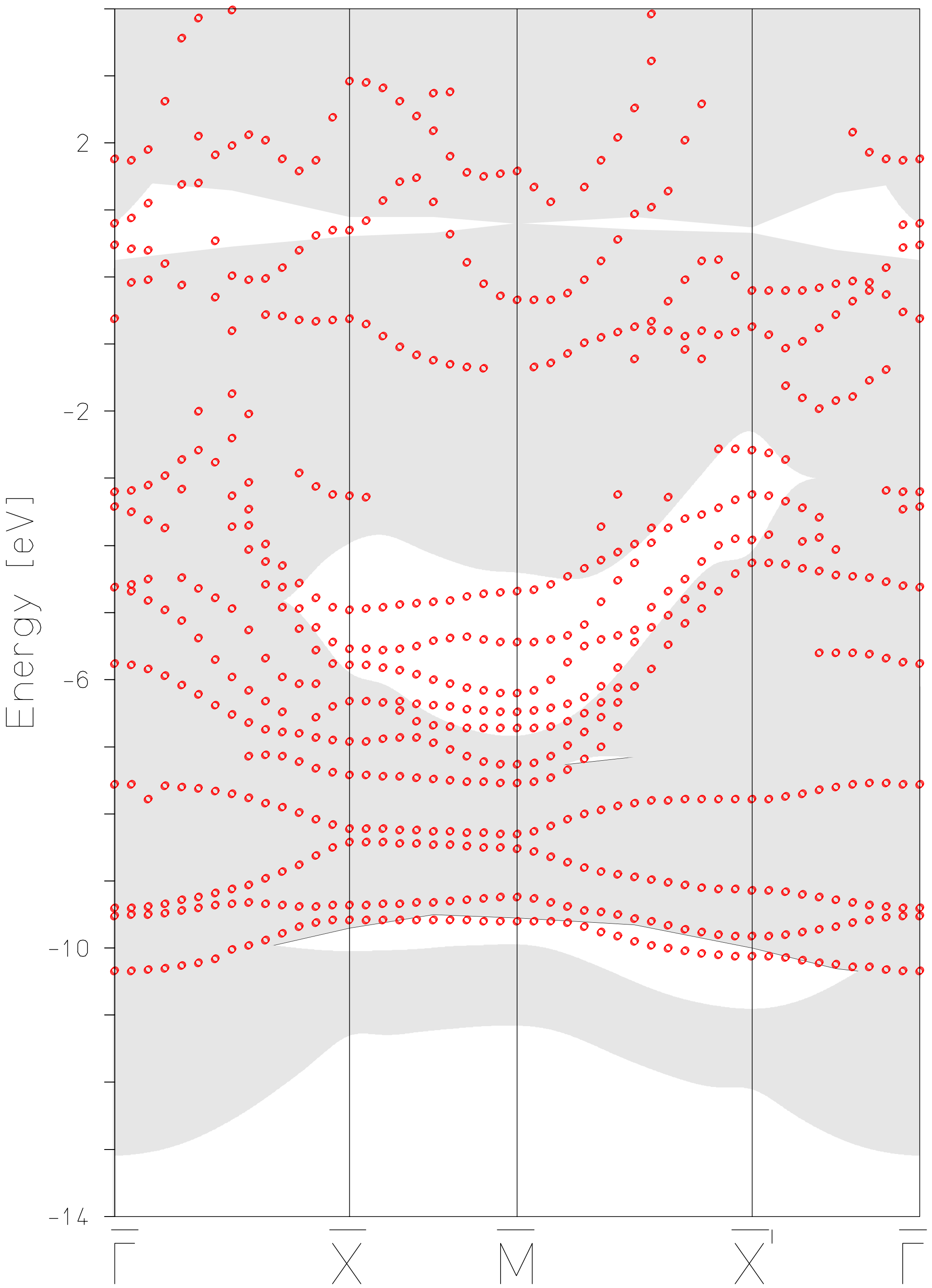

Figure 2: Surface electronic structure of the system GaAs(110)-p(1x1)-Sb(2L).

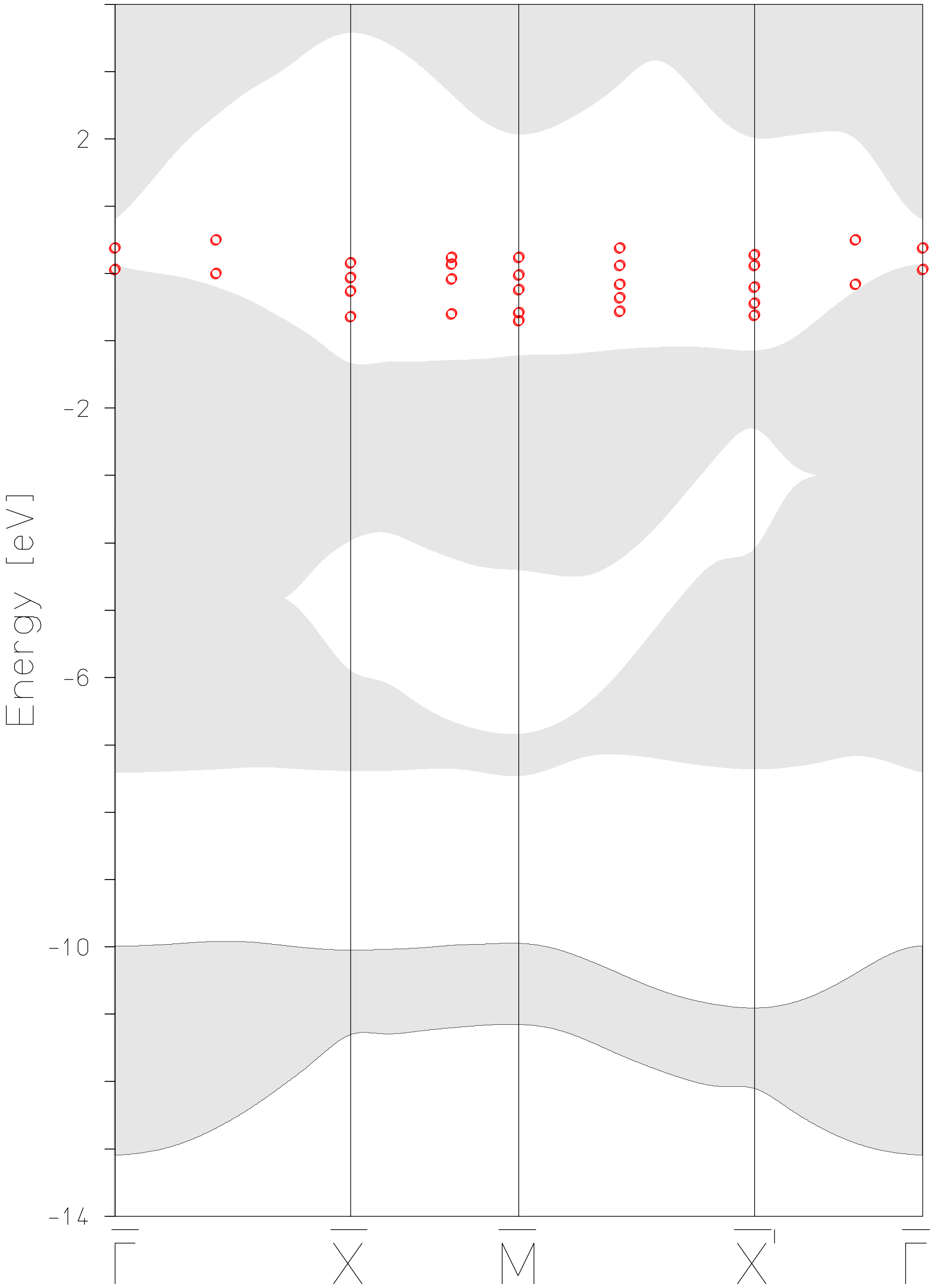

Figure 3: Interface states of the GaAs(110)/Sb(3L) system localized in the last GaAs layer.

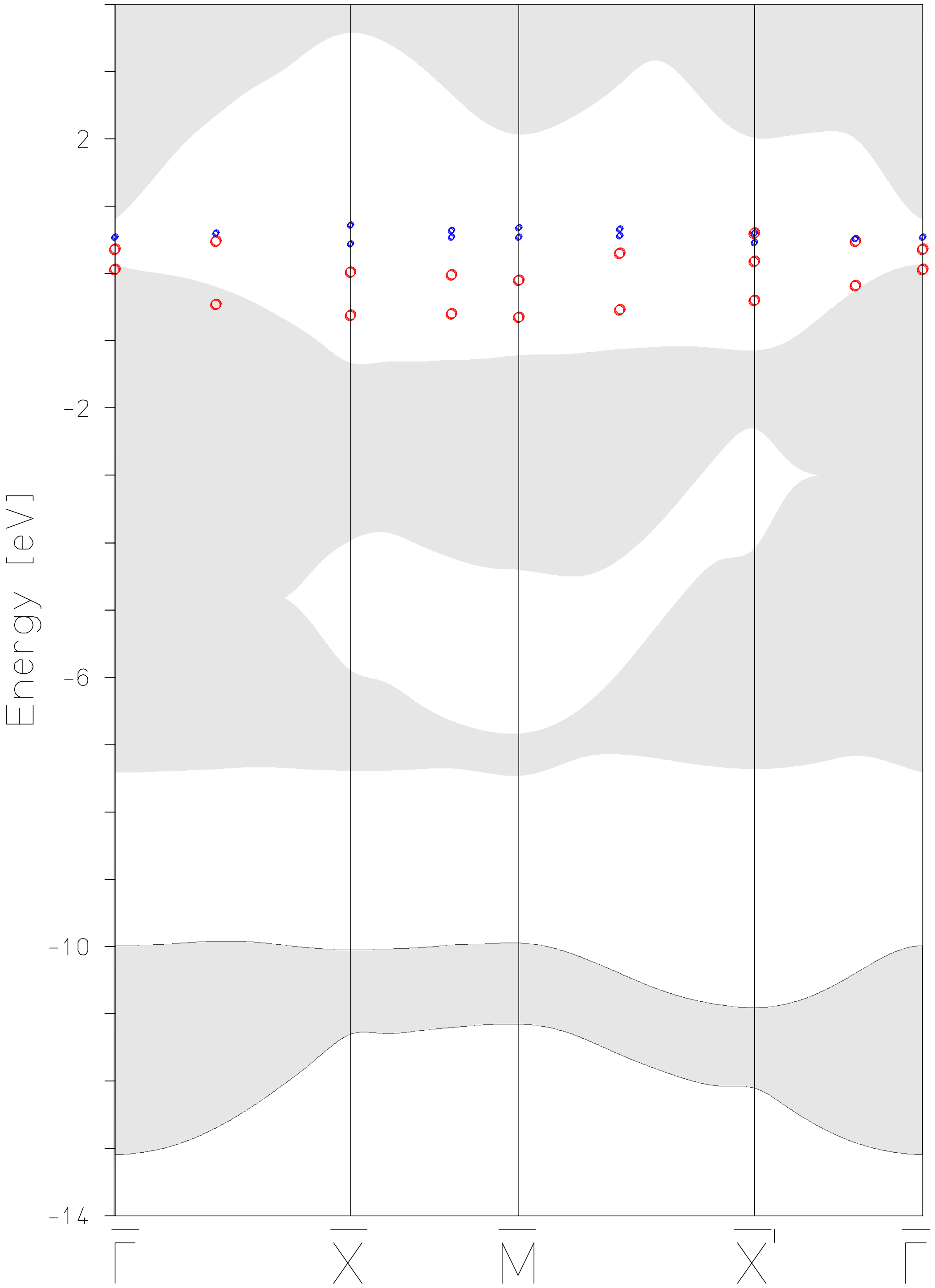

Figure 4: Interface states of the GaAs(110)/Sb system localized in the last GaAs layer (big red circles) and in the first Sb layer (small blue circles).

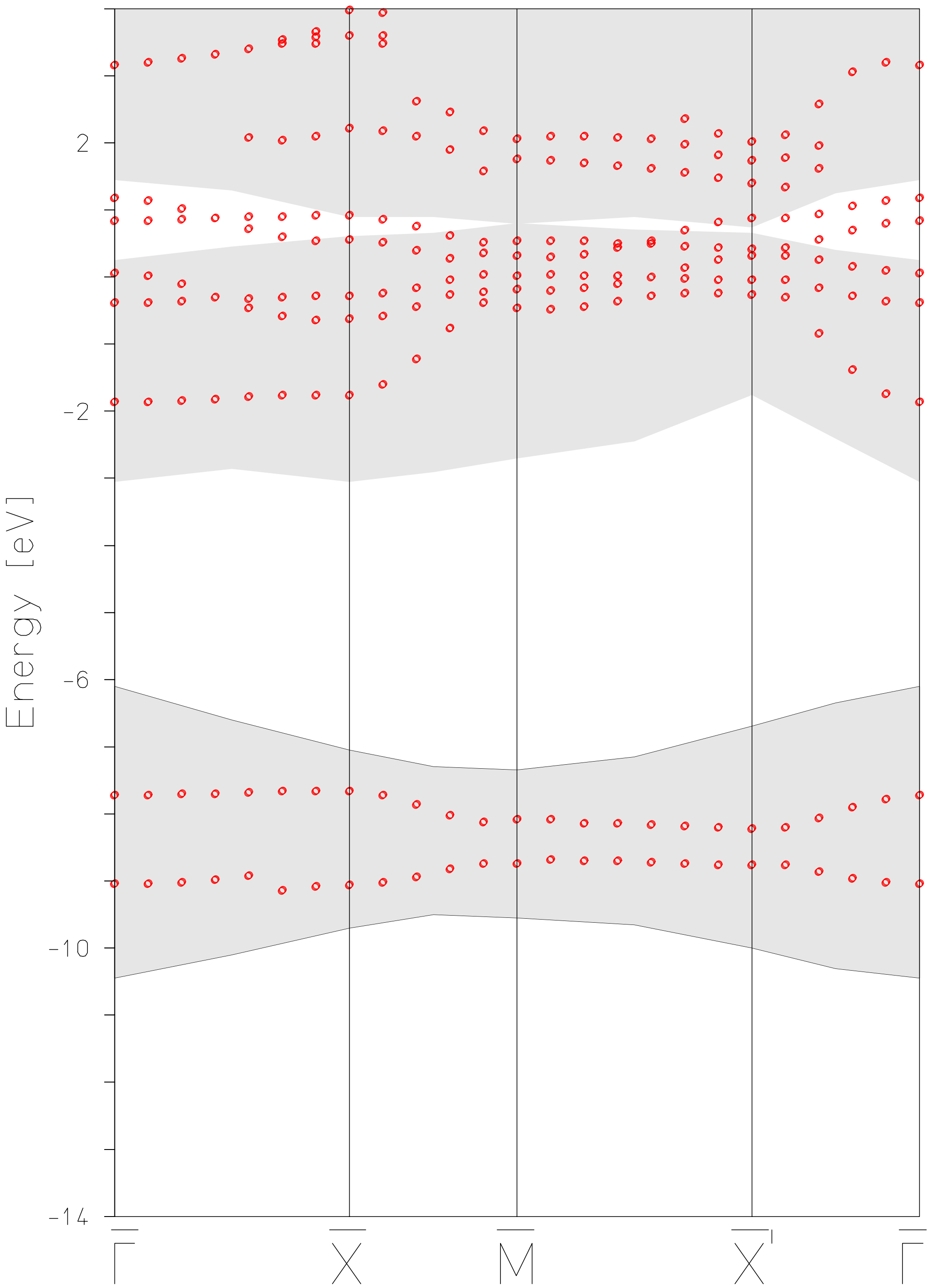

Figure 5: Surface electronic structure of the system GaAs(110)-p(1x1)-Sb(1ML)/Sb(1L).

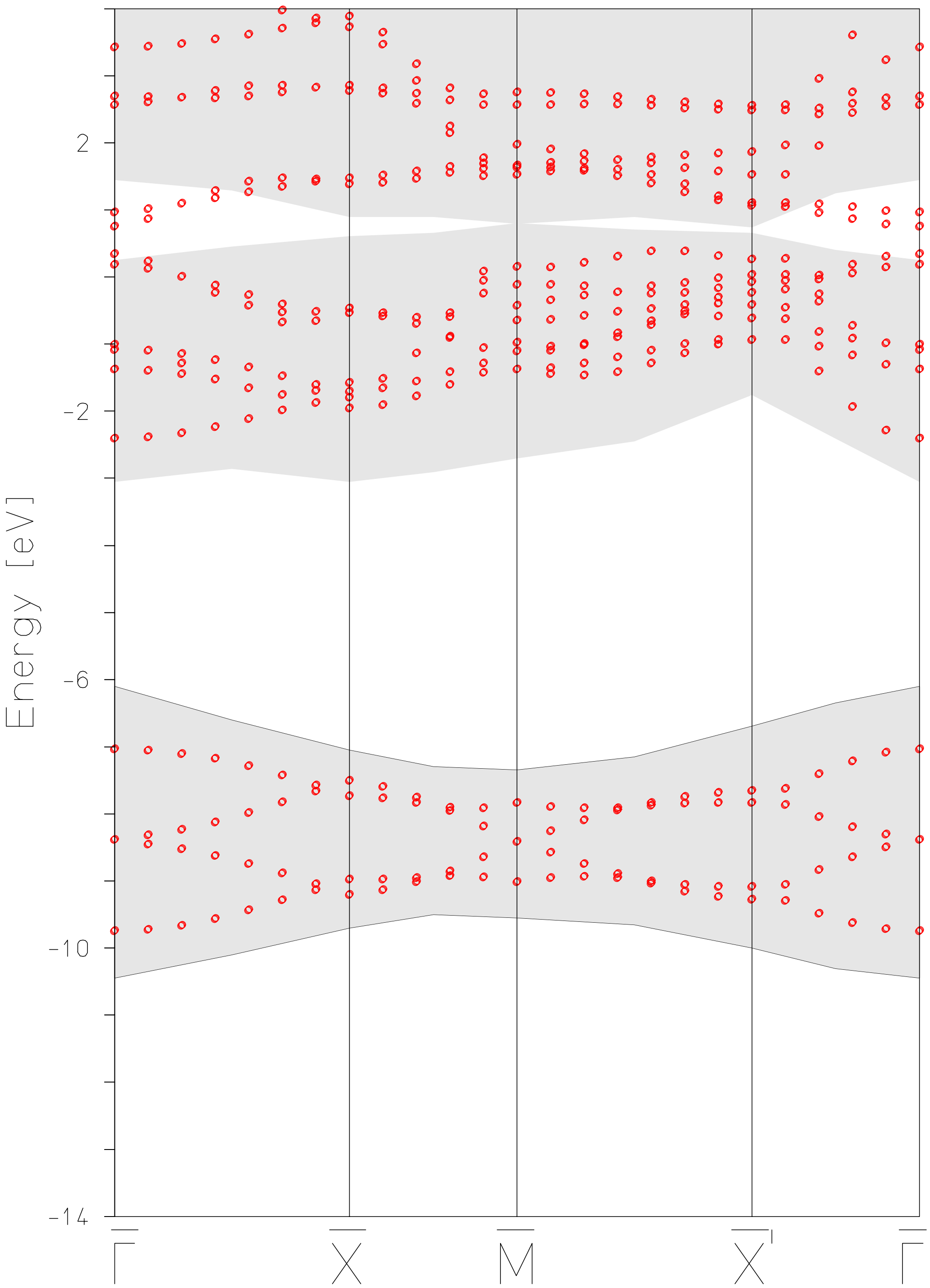

Figure 6: Surface electronic structure of the system GaAs(110) /Sb(2L).

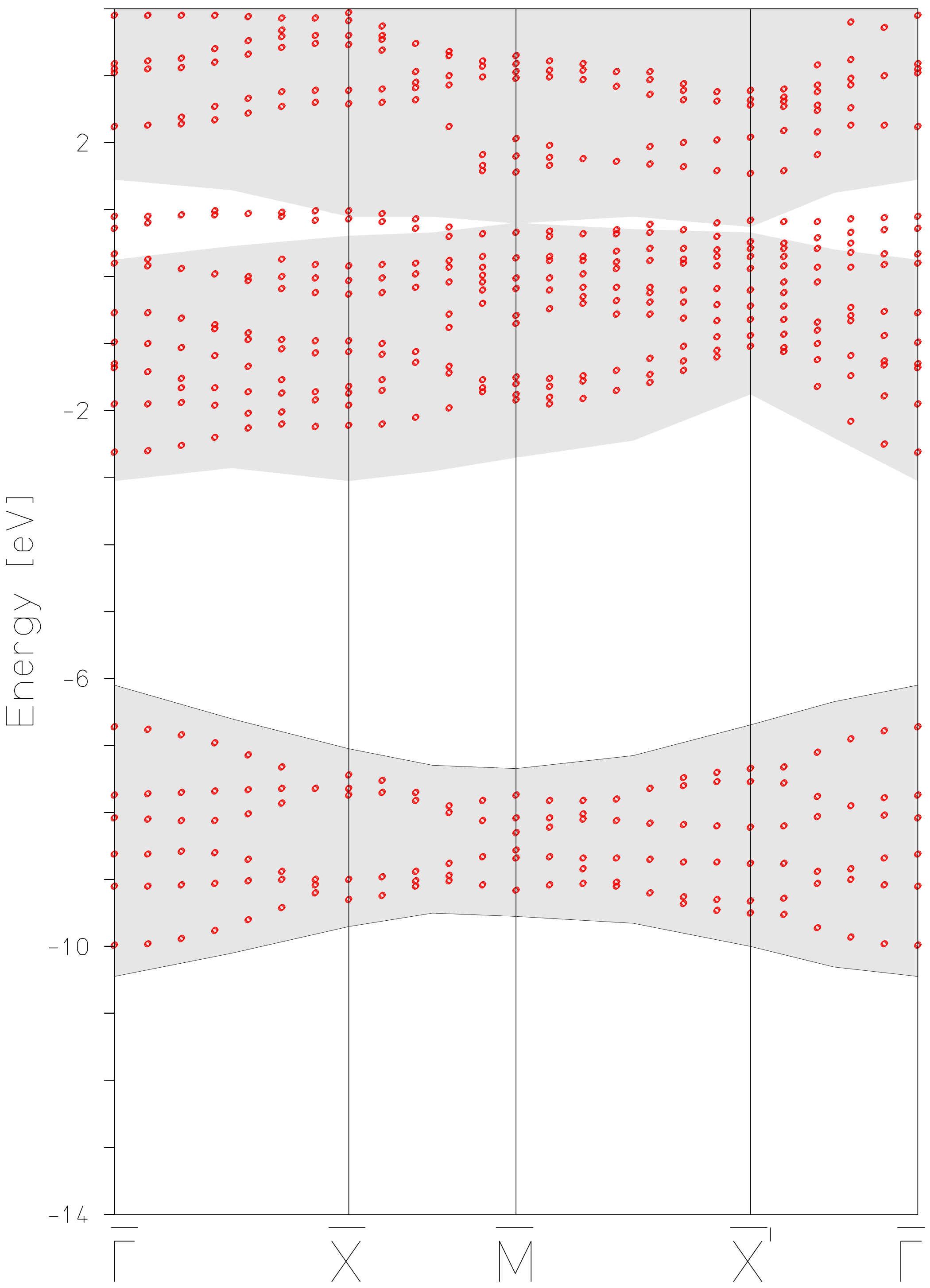

Figure 7: Surface electronic structure of the system GaAs(110) /Sb(3L).

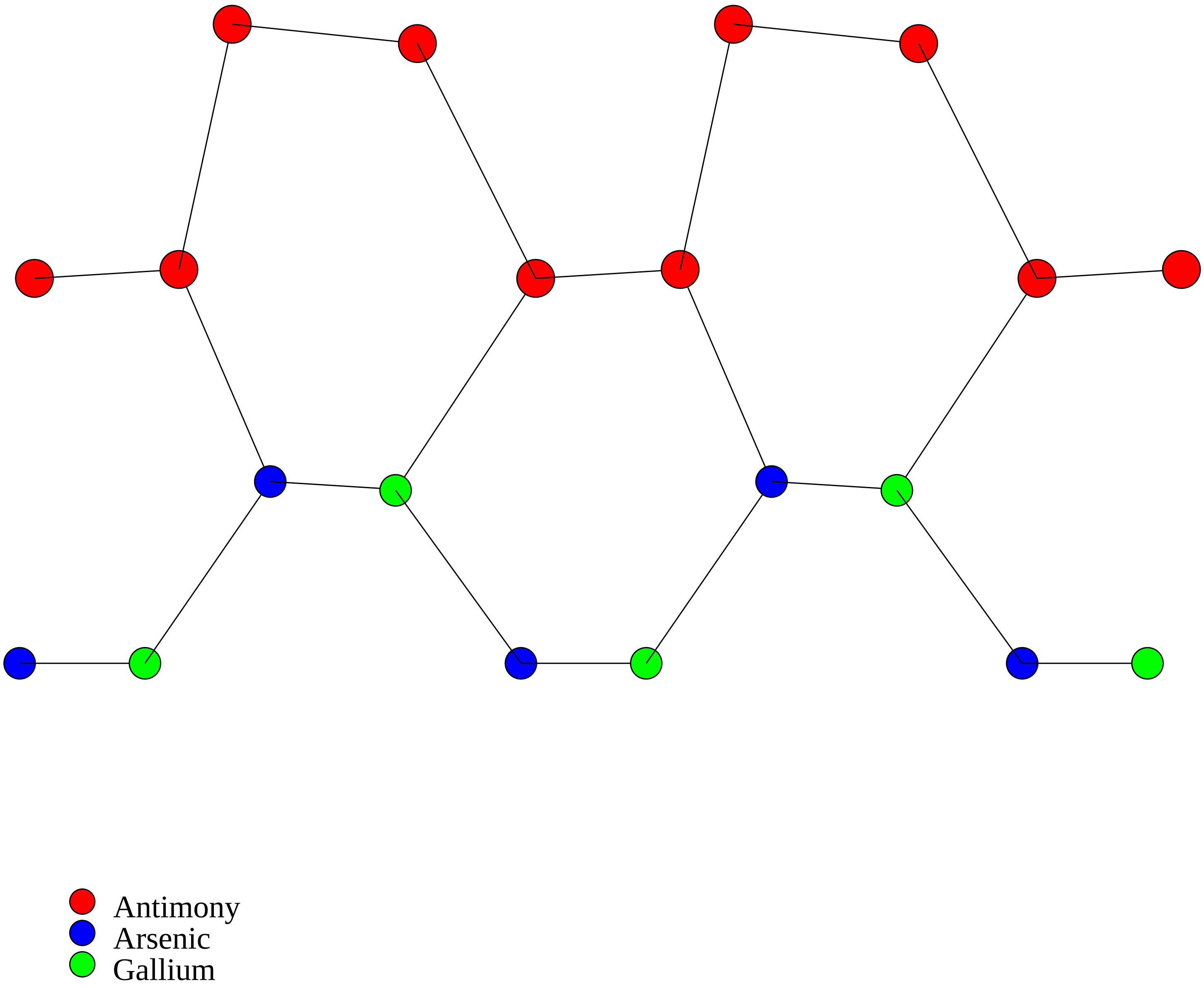

Figure 8: Atomic geometry of the GaAs(110)-p(1x1)-Sb(2L) system.

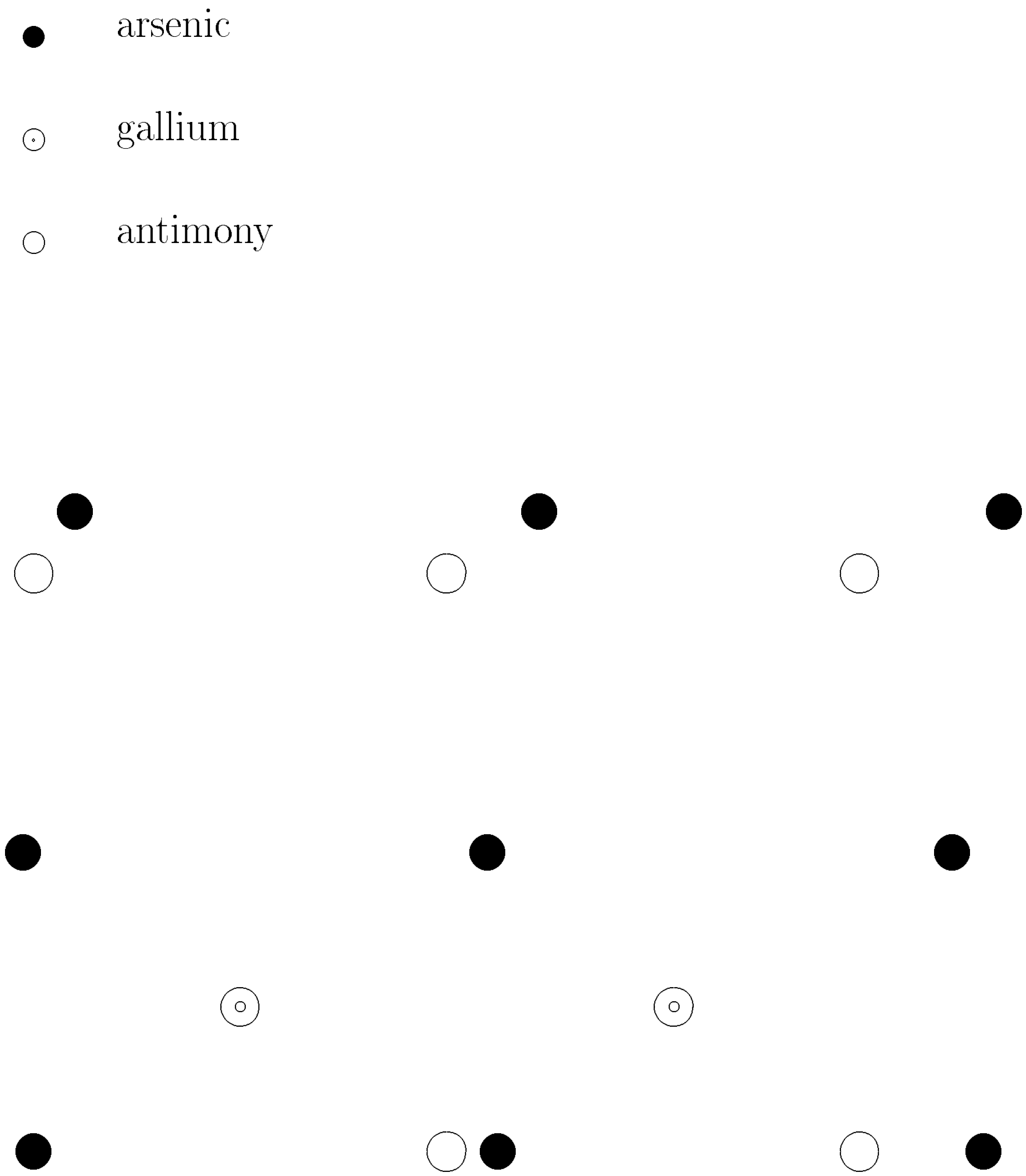

Figure 9: Atomic geometry of an ideal Sb layer (filled circles) in comparison with an ideal GaAs layer (empty circles).