The Fermi level is put to zero in all presented band structures in this work. As is seen, the conduction states at Fermi level and in the occupied region of the conduction bands have very small wavefunction amplitudes in the LaO layers (cf. Fig. 2 for the layered structure). As has already been stated many times, they have predominantly Fe-3d character and decay exponentially into the LaO layers. Experimentally it is found[5] that superconducting F-doped LaOFeAs shows an intrinsic Josephson effect like bismuth cuprate[6] which is only possible if the spacer layers are not metallic and form tunnel barriers instead. The band structure analysis of Fig. 1 indicates a conduction gap of several eV of the LaO layer. This is in contrast to $Ba(FeAs)_2$ where the Ba layers are obtained at least close to be metallic through Ba-5d orbitals.[4] Also seen in the figure by comparison of its left ($k_z = 0$) with its right part ($k_z = \pi$) is the pronounced two-dimensional (2D) character of the conduction states.

We calculated also the bands for the experimental structure parameters. The deformation potentials with respect to change of the lattice constants and of the Wyckoff parameters for the Fe-3d bands crossing the Fermi level are typically 2 eV/Å. Both band structures deviate from each other less than 0.2 eV in the window ±1 eV around Fermi level, which is irrelevant for our considerations. (The two nearly parallel dispersive bands along Γ-Z below Fermi level have Fe-3d_{z^2} character, which will appear even somewhat lower in energy if the experimental Wyckoff parameter is used instead of the GGA relaxed value (cf. Table I).) The unoccupied dispersionless La-4f bands are seen about 3 eV above Fermi level.

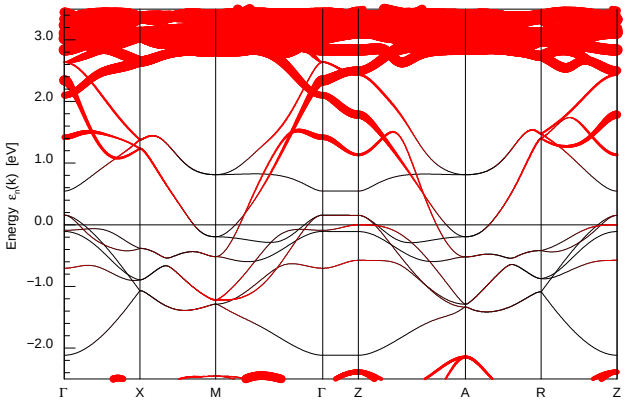

Figure 1: (color online) The Kohn-Sham GGA band structure of bulk LaOFeAs. The 'fat bands' in red weigh the O-2p and La-4$f, 5d, 6s$ orbital contribution to the band state.

First we want to learn something on the cleavage behavior and the layer bonding. To this goal, a periodic stacking of layers

As/Fe/As/La/O/La/As/Fe/As/La/O/La

is considered (in c-direction doubled unit cell). The symmetry is lowered in this case to the orthorhombic space group Pmm2 so that all atom layers have free z Wyckoff parameters. (In the space group P4/nmm of the bulk crystal the z Wyckoff parameters of O and Fe layers are fixed by symmetry to the values 0 and 1/2, respectively.) Now, for a sequence of increasing c lattice constants the z Wyckoff parameters of all atom layers were relaxed. As will be seen from the results presented in the next section, the crystal is expected to cleave between As and La layers only. Hence, clean coherent As or La surfaces are expected after cleavage. In a real crystal, due to defects of course terraces will likely be obtained consisting of coherent As and La terminated areas, respectively.

Next, two types of symmetrically terminated periodically repeated slabs with the full space group P4/nmm are considered with atom layer stacking

As/Fe/As/La/O/La/As/Fe/As/La/O/La/As/Fe/As

and

La/O/La/As/Fe/As/La/O/La/As/Fe/As/La/O/La

(Fig. 2) with sufficiently large space between terminating surfaces so that subsequent slabs do not interact any more. For stacks of symmetric slabs this is easily obtained if there is sufficient space for the electronic states not to overlap across the spacing: Due to symmetry there is no electric field in the free space between the slabs. Since there are two atoms per Fe and O layer in the unit cell and one of the other atoms per layer, the unit cells of these stacks are $(LaO)_4(FeAs)_6$ and $(LaO)_6(FeAs)_4$, respectively.

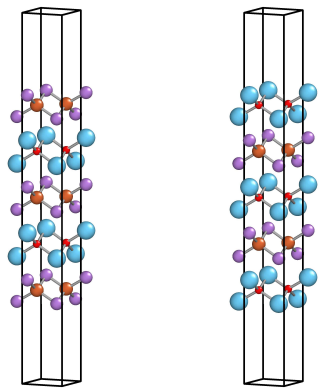

Figure 2: (color online) Slab geometry: unit cells of $(LaO)_4(FeAs)_6$ (left) and $(LaO)_6(FeAs)_4$ (right) slabs; blue: La, red: O, orange: Fe and violet: As

To check that the results are representative for surfaces of bulk crystals, both the spacing between the slabs and the slab thickness were varied. In addition to the above, $(LaO)_8(FeAs)_{10}$ and $(LaO)_{10}(FeAs)_8$ slabs are considered. Besides the results of structure relaxation, stability of layer charges is considered as a check for convergence of the considered slabs towards open bulk crystal surfaces. Given the total charge density of a crystal there is ambiguity to assign charges to the atom sites, and dif-