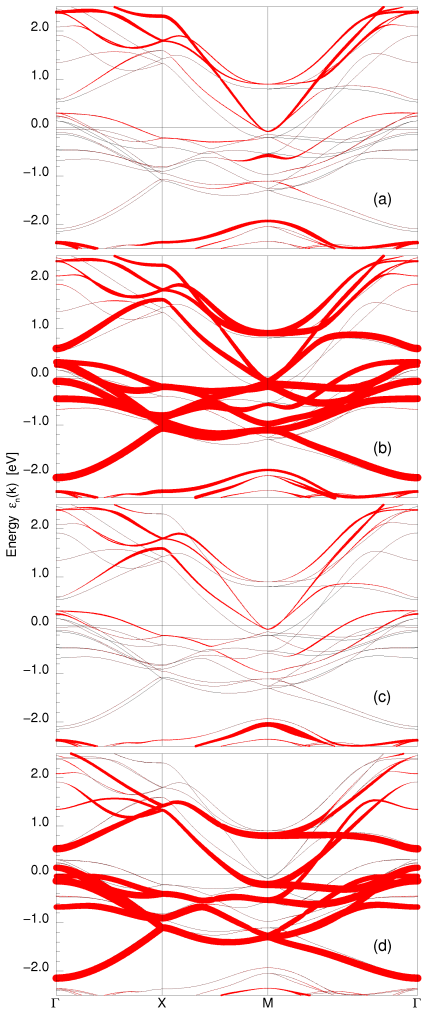

Figure 4: (color online) Band structure of the $(LaO)_4(FeAs)_6$ slab. The thickness of the red (shadow) lines represents in turn the orbital weight of (a) surface As 4p, (b) subsurface Fe 3d, (c) subsurface As 4p, and (d) central (bulk) Fe 3d.

C. The As terminated surface

As can be inferred from Tables II and III, the central Fe-As triple layer of $(LaO)_4(FeAs)_6$ is already close to a bulk-like state. Also the Fermi level relative to the bands derived from this central layer is bulk-like. Therefore, the band structure of this slab shown in Fig. 4 may be considered as representative for a bulk crystal with an As terminated (001) surface. Observe that the slab bands do not have k_z-dispersion due to the slab confinement of the Kohn-Sham states. As is seen in Fig. 1, the k_z-dispersion of the bulk bands crossing Fermi level is also negligible. Therefore, in the following only the in-plane dispersion of the bands is discussed and presented in the figures.

By the thickness of colored lines, the orbital character of the bands is indicated in Fig. 4 from top to bottom

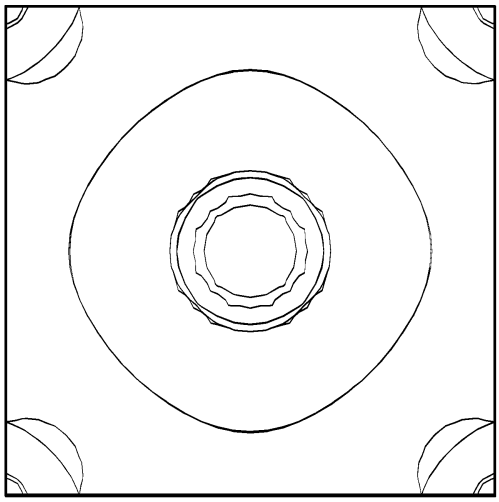

Figure 5: The 2D FSs of the slab $(LaO)_4(FeAs)_6$. The zone center is Γ and the corner point is M. From Γ outward in turn the FSs are: 2 times bulk, 3 times surface; from M outward: two tiny surface FSs, two bulk FSs. (The small wiggles are due to the resolution of the used $\boldsymbol{k}$ mesh.)

for basis orbitals in which the Kohn-Sham band wavefunctions are expanded: of surface As 4p-orbitals, Fe 3d-orbitals of the Fe layer below the surface As layer, As 4p-orbitals of the next layer below this Fe layer, and finally of the Fe 3d-orbitals in the center of the slab which corresponds to the first Fe layer below the surface triple layer of a bulk crystal. The latter Fe atoms are about 10 Å below the position of the surface As atoms.

The Kohn-Sham band wavefunctions in the vicinity of Fermi level are formed by the above accounted 'chemical basis' orbitals to about 99 percent so that the thick colored lines of Fig. 4 (and also of Fig. 6 below) completely represent the extension of the corresponding Kohn-Sham wavefunctions. Polarization states, and other basis states besides the explicitly discussed, of the full basis used in the calculations to not contribute to these Kohn-Sham wavefunctions.

Both the surface Fe 3d-bands and the bulk Fe 3d-bands cross the Fermi level, however, they form quite different Fermi surfaces (FS) as shown in Fig. 5. Around Γ there are two hole cylinders of bulk bands and around M there are two electron cylinders, all much like in a bulk crystal calculation without surface. Note that in the slab $(LaO)_4(FeAs)_6$ on which Fig. 5 is based the surfaces FSs are (almost) twofold degenerate due to the two surface FeAs triple layers on both sides of the slab (which do almost not interact due to the z-confinement of all conduction states). Hence, each of the surface FSs is doubly degenerate which is, however, not resolved in the figure.

There is next to no contribution of orbitals in the subsurface LaO triple layer as well as in any LaO triple layer