



FIG. 1: Energy bands of LaOFeAs, for the theoretically optimized (left) and experimental position (right) of the As atom, along various symmetry directions in the Brillouin zone. The upper panel highlights the region around the Fermi level. Dashed line in the upper panel indicates the position of the Fermi level for the 14% doped LaOFeAs.

of LaOFeAs calculated using both  $z_{\text{As}}$  are shown in Fig. 1. Four bands cross the Fermi level  $E_F$ , having predominantly Fe  $d$  character moderately hybridized with As  $p$ . These band structures are in agreement with previous results<sup>16,25</sup>.

The corresponding FS are given in Fig. 2. The FS calculated with optimized and experimental  $z_{\text{As}}$  for the undoped compound are quite similar with two  $e$ -like cylinders around the  $M$  point and two  $h$ -like cylinders warped around the  $\Gamma$  point of the BZ. However, the two FS differ when it comes to the third  $h$ -like manifold which appears as a 3D structure on the use of optimized As positions and as a 2D cylinder when the experimental atomic positions are used.

Since the parent compound becomes superconducting on electron doping, it is important to look at the change in the electronic structure as a function of the Fluorine content. The doping is treated by the means of rigid band model (RBM) which is a reasonable approximation for LaOFeAs<sup>28</sup>. As for the crystal structure, it is kept fixed to the undoped values even for the doped case. This choice is justified for the material under investigation; it was shown by Mazin et al.<sup>25</sup> that the lattice parameter and atomic positions are not sensitive to the doping. The FS for the 14% doped compound is shown in Fig. 2. Even though the undoped FS calculated using optimized and experimental  $z_{\text{As}}$  are substantially different, the doped FS for the two cases are fairly similar. The  $h$ -like FS sheet around  $\Gamma$  point for  $x = 0$  quickly disappears on electron doping in both cases ( $z_{\text{As}}$  optimized and experimental) with only 2D tubular structures around the  $\Gamma - Z$  ( $h$ -like) and the  $M - A$  ( $e$ -like) lines surviving.