

function of frequency are presented. Finally the conclusions are given in Section IV.

II. METHOD

The independent electron susceptibility is defined as:

$$\chi_0(\mathbf{q}, \mathbf{G}, \mathbf{G}', \omega) = \sum_{nn'\mathbf{k}} \frac{f_{n\mathbf{k}} - f_{n'\mathbf{k}+\mathbf{q}}}{\epsilon_{n\mathbf{k}} - \epsilon_{n'\mathbf{k}+\mathbf{q}} + \hbar(\omega + i\eta)} \langle n'\mathbf{k} + \mathbf{q} | \mathbf{e}^{i(\mathbf{q}+\mathbf{G})\cdot\mathbf{r}} | n\mathbf{k} \rangle \langle n\mathbf{k} | \mathbf{e}^{-i(\mathbf{q}+\mathbf{G}')\cdot\mathbf{r}} | n'\mathbf{k} + \mathbf{q} \rangle \quad (1)$$

where $\epsilon_{n\mathbf{k}}$ and $f_{n\mathbf{k}}$ are the one-electron energies and the corresponding Fermi functions, and \mathbf{G}, \mathbf{G}' are reciprocal lattice vectors. In this work we accurately compute χ_0 by performing the summations in Eq. (1) using a random sampling over the Brillouin zone (BZ). We used ~ 3000 independent \mathbf{k} -points per band, chosen according to a stochastic algorithm which accumulates them around the FS for bands crossing E_F . The final results are obtained by averaging over 40 runs each containing completely independent \mathbf{k} -point set. This procedure nearly completely eliminates the numerical noise, and shows a good convergence both in terms of number of independent runs and number of \mathbf{k} -points within a single run. We have included 65 bands in order to ensure convergence with respect to the number of empty bands.

The energy bands and the matrix elements for LaOFeAs have been calculated, within the (spin-independent) local density approximation (LDA)²⁴ to the exchange-correlation functional. Our calculations have been done using the Full-potential Linearized Augmented Plane Wave (FPLAPW) method. This choice is necessary because of the extreme sensitivity of the electronic structure (in particular, of the bands close to E_F) to the method²⁵. No numerical approximation has been made in the evaluation of matrix elements in Eq. (1). Given the huge debate about the dependence of the results on the position of the As atom in the unit-cell^{25,26}, in the present work we show results both for the theoretically optimized ($z_{\text{As}} = 0.638$) and experimental²⁷ ($z_{\text{As}} = 0.6513$) position of the As atom.

III. RESULTS AND DISCUSSION

We first look at the band structure and the FS for the parent and the doped LaOFeAs. The ground state calculations are performed with the tetragonal unit cell, containing two Fe atoms, at the experimental lattice constants $a = 4.03\text{\AA}$ and $c/a = 2.166$. The energy bands