



FIG. 6: Real part of  $\chi(\mathbf{q}, 0)$  on the basal plane (i.e.  $q_z = 0$ ), calculated using the experimental position of the As atom. Top-panel: (a) for the undoped case and (b) for the 14% doped case. Bottom-panel: (c) difference between (a) and same calculated at the theoretically optimized position of the As atom and (d) difference between (b) and same calculated at the theoretically optimized position of the As atom.

the flat La  $4f$  bands visible at around 3 eV in Fig. 1 do not result into any evident structure in the  $\text{Im}\chi_0$  plot, indicating the small hybridization (thereby small matrix element) of these states with Fe and As states.

At small values of  $\mathbf{q}$  and at low frequency, the value of  $\text{Im}\chi_0$  grows linearly as a function of the frequency and then drops rapidly to zero (resembling linear response susceptibility for the non-interacting electron gas). From Fig. 7(a), we see that this low frequency feature has two components; the position of the first peak grows with  $\mathbf{q}$ , saturating at a frequency of  $\sim 0.4$  eV, while the second one grows up to  $\sim 1$  eV finally merging into the main broad peak. This behaviour is the same along the  $\Gamma - M - \Gamma$  and  $\Gamma - X - \Gamma$  lines, except for the presence of an extra low frequency structure ( $\omega \leq 0.3$  eV) visible around the  $M$ -point. A detailed view of  $\text{Im}\chi_0(\mathbf{q}, \omega)$  and the behaviour of  $\text{Re}\chi_0(\mathbf{q}, \omega)$  is given in Fig. 7(b) at  $X$  and  $M$ , both for the undoped and for the doped systems. Even though doping does not significantly change the general shape of both real and imaginary parts of  $\chi_0$ , in the low frequency region, we notice a different behaviour of  $\text{Im}\chi_0(\mathbf{q}, \omega)$  at  $M$  (see inset of Fig. 7b). For  $x = 0$  the  $\text{Im}\chi_0$  grows linearly as a function of  $\omega$ , while it only starts to grow at a finite value of  $\omega$  for  $x = 0.14$ . The reason for this is closely tied to the nesting function; An highly nested FS gives rise to linear behaviour for  $x = 0$ . While in the doped case, deterioration of FS nesting at  $M$ , only allows finite energy excitations, leading to a finite starting value for