well with the experimental ones.

Fig. 2 shows the calculated Fermi surface cuts for LaOFeP and LaOFeAs on different $k_z$-planes based on the experimental lattice structures. The figure is almost unchanged if we consider the optimized lattice structure. The hole Fermi surfaces around $(0, 0, k_z)$ are shifted by $(\pi, \pi, 0)$ to show the nesting properties. Shifting of $(\pi, \pi, \pi)$ was also investigated, and we find that the nesting properties are nearly unchanged. From the figure, it is apparent that the Fermi surface nesting is even more perfect in LaOFeP than in LaOFeAs, indicating a stronger tendency to stripe-type antiferromagnetic ordering in LaOFeP compared to LaOFeAs. However, experimentally, while a small magnetization is observed in undoped LaOFeAs[77], superconductivity rather than magnetic order is detected in undoped LaOFeP[90]. These observations would indicate that Fermi surface nesting might not be connected to magnetization.

In order to quantify the Fermi surface nesting, we show in Fig. 3 the $\mathbf{q}$-dependent Pauli susceptibilities at fixed $q_z = \pi$ for LaOFeP and LaOFeAs with subtraction of the corresponding values at $\mathbf{q}_0 = (0, 0, \pi)$. While a peak in LaOFeP appears right at $\mathbf{q}_\pi = (\pi, \pi, \pi)$ indicating almost perfect nesting properties of the Fermi surfaces, peaks are situated close to $\mathbf{q}_\pi = (\pi, \pi, \pi)$ in LaOFeAs suggesting nearly nested Fermi surfaces, which is consistent with the Fermi surface cuts shown in Fig. 2. The most interesting finding in Fig. 3 is that the relative values $\chi(\pi, \pi, \pi)$-$\chi(0, 0, \pi)$ increase from LaOFeP to LaOFeAs irrespective of whether the Fermi surface nesting is perfect or not. While the peak at $(\pi, \pi, \pi)$ favors stripe-type antiferromagnetic ordering, the one at $(0, 0, \pi)$ represents a possible instability towards checkerboard-type antiferromagnetic ordering or A-type antiferromagnetic ordering where ferromagnetic layers are stacked antiferromagnetically. The heights of these two peaks become closer in LaOFeP than in LaOFeAs, implying that competition between the above-mentioned two types of antiferromagnetic states becomes stronger in LaOFeP if thermal or quantum fluctuations are taken into account. Also spin-fluctuation mediated pairing of the superconducting state[23,26,30] coming from inter-band scattering around $\mathbf{q}_\pi = (\pi, \pi, \pi)$ takes part in the competition. Eventually, as the two types of antiferromagnetism strongly compete with each other, the additional superconducting state order emerges and opens a gap, removing the high instability at the Fermi level and lowering the total energy. This could be the scenario to explain why undoped LaOFeP is always nonmagnetic but shows superconductivity below 3.2 K at ambient pressure. As $\chi(\pi, \pi, \pi) - \chi(0, 0, \pi)$ increases beyond a critical value, the stripe-type antiferromagnetic ordering prevails over the checkerboard-type one and the pairing. This scenario may apply to the low-temperature magnetic phase of LaOFeAs. Furthermore, we have calculated the total energies of checkerboard and stripe-type antiferromagnetic phases for both LaOFeP and LaOFeAs. We found that the stripe-type antiferromagnetic phases are the ground state in both

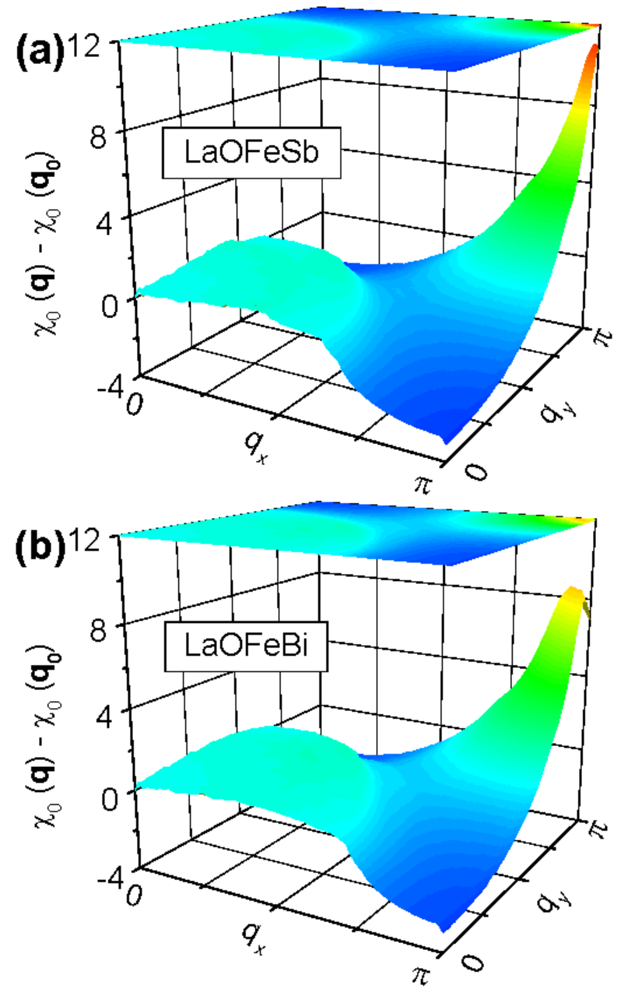


FIG. 4: (Color online) Static $\mathbf{q}$-dependent Pauli susceptibilities at fixed $q_z = \pi$ for (a) LaOFeSb and (b) LaOFeBi. The corresponding values of the Pauli susceptibilities at $\mathbf{q}_0 = (0, 0, \pi)$ in LaOFeSb and LaOFeBi, respectively, are subtracted. On top, two-dimensional contour maps are shown. In the DFT calculations GGA is used.

cases and the energy difference between the two phases is smaller in LaOFeP than in LaOFeAs, which is consistent with the trend of $\chi(\pi, \pi, \pi)$-$\chi(0, 0, \pi)$.

In Fig. 4, we display the $\mathbf{q}$-dependent Pauli susceptibilities at fixed $q_z = \pi$ for the hypothetical compounds LaOFeSb and LaOFeBi. The corresponding values of the Pauli susceptibilities at $\mathbf{q}_0 = (0, 0, \pi)$ in LaOFeSb and LaOFeBi, respectively, are again subtracted. Note that $\chi(\pi, \pi, \pi) - \chi(0, 0, \pi)$ in LaOFeSb and LaOFeBi is even larger than that in LaOFeAs (see Fig. 3), indicating that the instability towards stripe-type antiferromagnetic ordering could win the competition between different instabilities in these two compounds. It is also interesting to note that the peak at $\mathbf{q}_0 = (0, 0, \pi)$ becomes flatter when we go from LaOFeP to LaOFeBi. While the flatness of the peak can be associated with a larger number of different magnetic structures lying