FIG. 1: (Color online) Comparison of normalized static **q**-dependent Pauli susceptibilities at fixed $q_z = \pi$ between arsenide and antimonide of (a) 111 compounds, (b) 1111 compounds and (c) 122 compounds. The normalization factors are the susceptibilities of the corresponding arsenide systems for each type of compound at $\mathbf{q}_0 = (0, 0, \pi)$. Please note that the peak position is not exactly at $\mathbf{q}_\pi = (\pi, \pi, \pi)$ since the electron and hole Fermi surfaces are nearly nested rather than perfectly nested. Here, GGA is used for the DFT calculations.

magnetic metallic states and magnetic moments increase with the substitution of As by Sb in LaOFeAs, BaFe$_2$As$_2$ and LiFeAs.

However, the magnetic moments we obtained are 1.6 (2.3) μ_B in LiFeAs (LiFeSb), 2.0 (2.5) μ_B in BaFe$_2$As$_2$ (BaFe$_2$Sb$_2$) and 1.8 (2.2) μ_B in LaOFeAs (LaOFeSb)[76], which are notably smaller than those obtained from the pseudopotential method[65,87]. Further comparing the optimized lattice structures, we find that, while our results are in good agreement with

TABLE I: Comparison between different DFT codes of the structures of LiFeAs optimized within GGA. z_{Li}=0.3385 and z_{As}=0.7688 are obtained from our CP-PAW calculations.

	a(Å)	b(Å)	c(Å)	$m(\mu_B)$	$d_{\text{Fe-As}}$(Å)
SIESTA[65]	5.482	5.285	6.190	2.54	2.434
VASP[85]	5.408	5.294	6.237	1.5	2.359
WIEN2k[86]	-	-	-	1.58	2.382
CP-PAW	5.422	5.307	6.255	1.56	2.385

previous GGA calculations, such as LiFeAs calculated with VASP[85] and WIEN2k[86], there are large differences between our results and those of Refs. 65,87 as shown in Table I. Furthermore, in Table II, we show the comparison between experimental and optimized structural data for BaFe$_2$As$_2$, where we find that our optimized structure agrees with the experimental one better than that from Ref. 65. Since the electronic band structure close to the Fermi level is sensitive to the lattice structure[20,88], the conclusion of Ref. 65 based on their optimized structures that there is no connection between Fermi surface nesting and magnetism is questionable. Therefore, we reinvestigate the nesting property of the Fermi surface.

TABLE II: Comparison between the experimental structure of BaFe$_2$As$_2$ and the optimized structures from different DFT codes within GGA. The magnetic moment on each Fe is also shown. z_{As}=0.6495 is obtained from our CP-PAW calculations.

	a(Å)	b(Å)	c(Å)	$m(\mu_B)$	$d_{\text{Fe-As}}$(Å)
Exp.[78]	5.616	5.571	12.943	0.87	2.392
SIESTA[65]	5.756	5.590	13.04	2.78	2.436
CP-PAW	5.693	5.666	13.008	1.98	2.396

Fig. 1 presents the comparison of normalized **q**-dependent Pauli susceptibilities at fixed $q_z = \pi$ between arsenides and antimonides in 111, 1111 and 122 compounds. The normalization factors are the susceptibilities of the corresponding arsenide for each type of compounds at $\mathbf{q}_0 = (0, 0, \pi)$. We fix $q_z = \pi$ because of the fact that spins on iron are arranged antiferromagnetically along the z direction as observed in experiments[77–81]. However, we checked that the conclusion drawn below will not be changed if $q_z = 0$ is fixed.

We find that in all Fe-based families, the situation is similar. Two peaks around $\mathbf{q}_0 = (0, 0, \pi)$ and $\mathbf{q}_\pi = (\pi, \pi, \pi)$ are detected in both arsenides and antimonides, and the peaks around (π, π, π) are always stronger than those around $(0, 0, \pi)$, indicating that the instability towards stripe-type antiferromagnetic ordering dominates, which is consistent with our spin-polarized GGA calculations. Most importantly, we find that, in contrast to Ref. 65, the Pauli susceptibilities are also enhanced together with the magnetizations when As is substituted by Sb in LaOFeAs, LiFeAs and BaFe$_2$As$_2$, which demon-