Supplemental material to the article

Electronic structure of NaFeAs superconductor: LDA+DMFT calculations compared with ARPES experiment

In this Supplement we provide more results of our calculations for other symmetry directions in the Brillouin zone and some additional comparisons with ARPES experiments at different polarizations.

In some sense MXM direction shown in Fig. 1 is the simplest one among others since only few bands are present here. The most intensive region here is around X point. For $k_z = \pi$ $3z^2 - r^2$ band goes a bit down in energy (panel f). It leads to lowering of intensity around X point for theoretical spectral function (panel e) and quantitatively reproduce ARPES data at 160 eV (panel d).

In Fig. 2 for XΓX high symmetry direction qualitative picture of bands evolution from $k_z = 0$ to π is the same as for MΓM direction (see Fig. 5 in the main text). Again the ARPES data at 80 eV (panel c) agrees better with $k_z = 0$ LDA+DMFT results (panels a and b). Most intensive spots of spectral function are formed at the crossing of xz, yz branches at -0.1 eV. While for $k_z = \pi$ most intensive region appears around -0.2 eV, where $3z^2 - r^2$ and xz, yz bands are dominating.

To discuss different Fe-3d orbitals contribution to spectral function maps we used experimental ARPES spectral functions obtained for different polarizations [24]. In Fig. 3 panel a corresponds to vertical polarization ARPES data in the MΓM high symmetry direction taken at 160 eV and panel f – to horizontal polarization. For vertically polarized beam "cap"-like structure around Γ-point is formed mainly by xz, yz orbitals (panels b and d for LDA+DMFT results). Surprisingly the intensity of xy band (panels c and e) is quite low in ARPES data and even not addressed in Ref. [24]. The k_z dispersion of these bands near the Fermi level is almost absent.

Horizontally polarized beam (panel f) wipes out $3z^2 - r^2$ band forming "M"-like structure around -0.2 eV. For $k_z = \pi$ it has higher intensity than for $k_z = 0$. It is in better agreement with to 159 eV data.

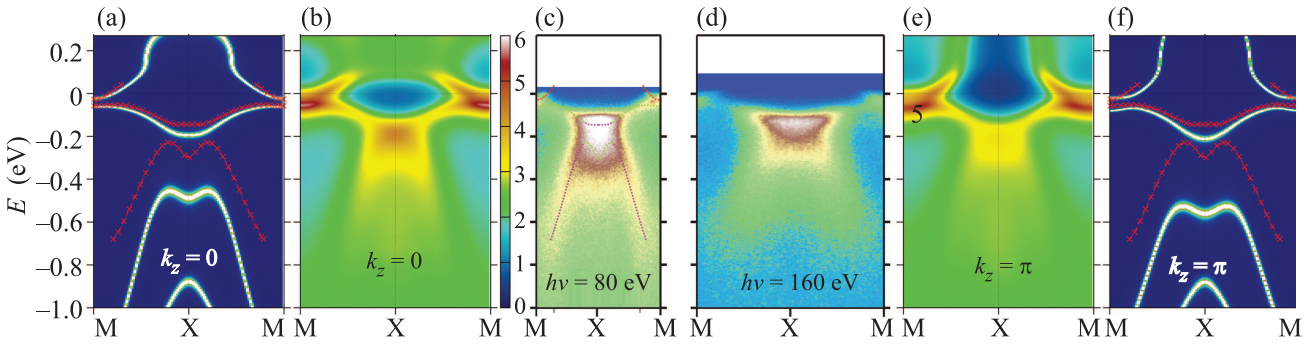

Figure 1: Comparison of experimental ARPES (panels c and d) [24] and LDA+DMFT (panels b and e) spectral functions in the MXM high symmetry direction for NaFeAs near the Fermi level. On the panels a and f experimental (crosses) [24] and theoretical (white lines) maxima dispersions of spectral functions are presented. The Fermi level E_{F} is at zero energy

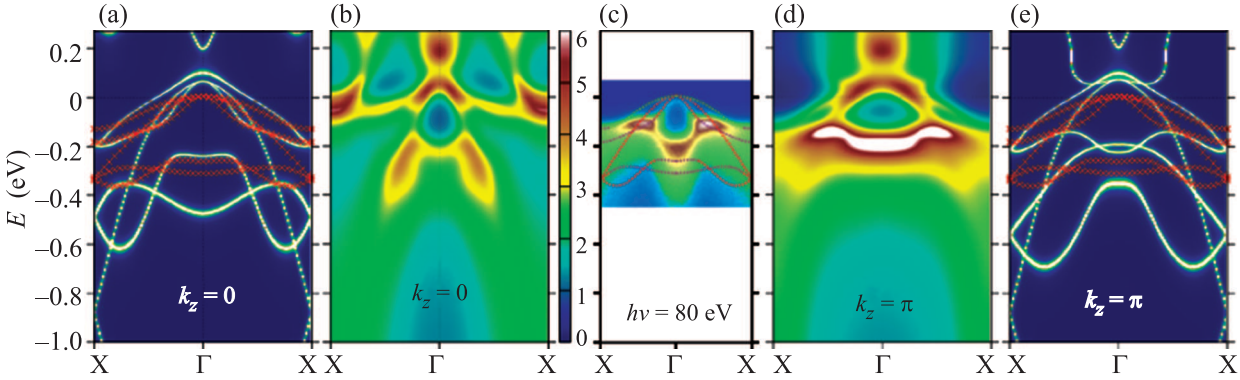

Figure 2: Comparison of experimental ARPES (panels c and d) [24] and LDA+DMFT (panels b and e) spectral functions in the XΓX high symmetry direction for NaFeAs near the Fermi level. On the panels a and e experimental (crosses) [24] and theoretical (white lines) maxima dispersions of spectral functions are presented. The Fermi level E_{F} is at zero energy

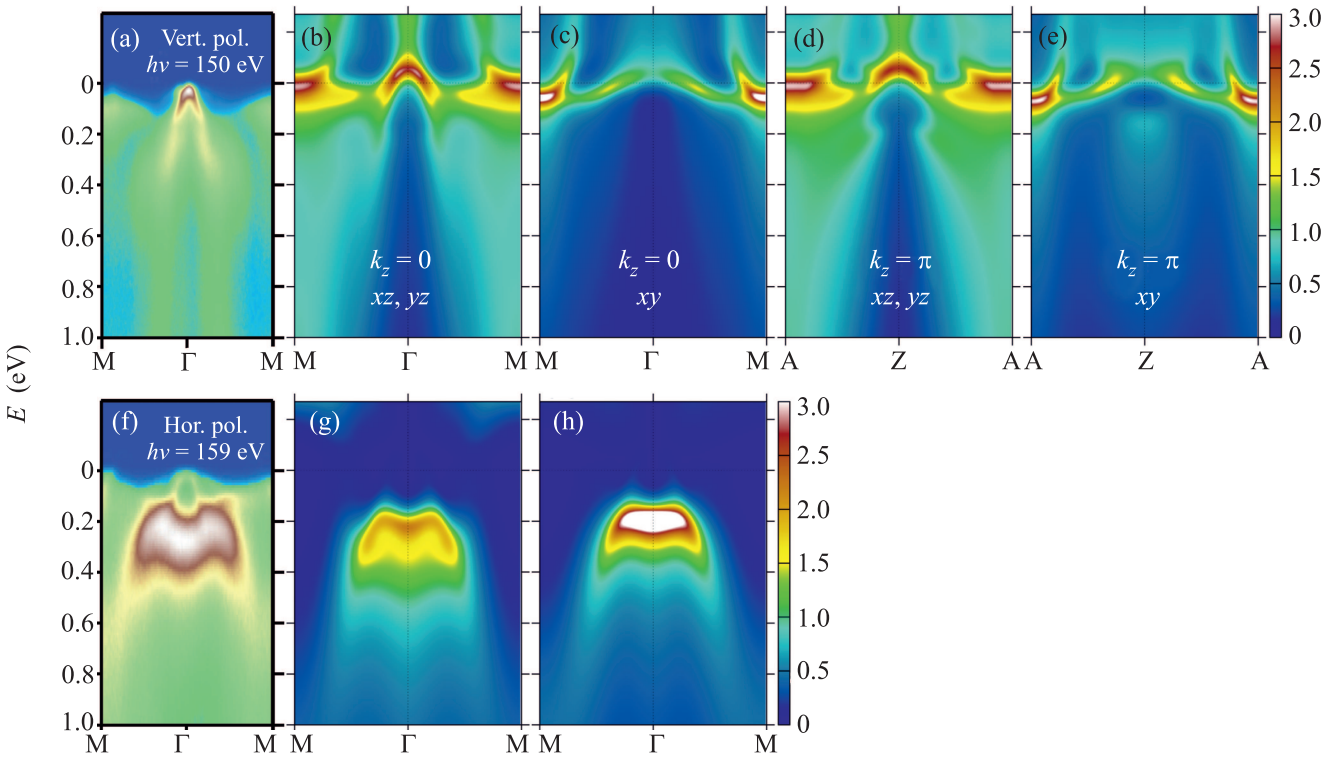

Figure 3: Comparison of experimental ARPES spectral functions with different polarization(panel a – vertical polarization, panel f – horizontal polarization) [24] and LDA+DMFT spectral functions for different Fe-3d orbitals: panels b–e – xz, yz, and xy contributions, panels g and h – $3z^2 - r^2$ contribution in the MΓM high symmetry direction for NaFeAs near the Fermi level for $k_z = 0$ and $k_z = \pi$ cases. The Fermi level E_{F} is at zero energy