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On the origin of the shallow and "replica" bands in FeSe monolayer superconductors[1)]

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ARPES measurements [1] in FeSe/STO monolayer system demonstrated rather unusual band structure, characterized by the absence of hole-like bands at the center of Brillouin zone (Γ-point), with rather shallow electronic band at the M-point with very low Fermi energies of the order of 50 meV, accompanied by the formation of "replica" of this band about 100 meV below in energy. Similar unusually shallow bands were also observed at X-point in ARPES experiments on intercalated $K_xFe_{2-y}Se_2$ system [2].

The existence of such peculiar bands rises many serious theoretical questions [3], such as probable considerable role of non-adiabatic interactions [4, 5] and the possibility of observation of BCS-BEC crossover effects in these systems. In particular, the formation of the "replica" band in FeSe/STO is widely interpreted as being due to interaction with high-energy (~ 100 meV) optical phonons of $Sr(Ba)TiO_3$ substrate [1] with some important conclusions on the possible role of these interactions for the significant enhancement of T_c in this system [4–7].

In Fig. 1 we compare the theoretical LDA+DMFT results on panels (a,d,e,h) with experimental ARPES data [1] on panels (b,c,f,g). LDA+DMFT spectral function maps of isolated FeSe monolayer are shown in Fig. 1a and Fig. 1d at Γ and M points respectively. For FeSe/STO LDA+DMFT spectral function maps are shown on e, h panels at Γ and M points.

Most of features observed in the ARPES data (Fig. 1f, g) can be identified with our calculated LDA+DMFT spectral function maps (Fig. 1e, h). The experimental quasiparticle bands around M-point marked by A, B, and C (Fig. 1g, h) correspond mainly to Fe-3d$_{xz}$ and Fe-3d$_{yz}$ states, while the A' and B' quasiparticle bands have predominantly Fe-3d$_{xy}$ character. As we noted above the appearance of A' band in FeSe/STO is usually attributed to forward scattering interaction with 100 meV optical phonon of STO substrate [1, 4–7]. However, our calculations show that A' band is most probably of purely electronic nature. Some puzzling behavior of this band can be explained by difficulties of experimental observations of the Fe-3d$_{xy}$ states near M-point (see Refs. [2, 8] and references therein, as well as Ref. [9]).

Thus, in FeSe/STO we observe the overall agreement between LDA+DMFT results (Fig. 1h) and ARPES data [1] (Fig. 1g) on semi-quantitative level with respect to relative positions of quasiparticle bands. Let us also note that the Fermi surfaces formed by the A and A' bands in our LDA+DMFT calculations are nearly the same as the Fermi surface observed at M-point by ARPES.

The shallow band at M-point originates from LDA Fe-3d$_{xz}$ and Fe-3d$_{yz}$ bands compressed by electronic correlations. In the hope of achieving the better agreement with experiments we also examined the reasonable increase of Coulomb interaction within LDA+DMFT and the different doping levels, but these have not produced the significant improvement of our results.

The C quasiparticle band near M-point appeared because of the lifting of degeneracy of Fe-3d$_{xz}$ and Fe-3d$_{yz}$ bands (in contrast to isolated FeSe layer, see panel Fig. 1d). The origin of this band splitting is related to the z_{Se} height difference below and above Fe ions plane due to the presence of interface with $SrTiO_3$.

Actually, all quasiparticle bands in the vicinity of M-point can be well represented as LDA bands compressed by a factor of 3 due to electronic correlations.

Our results essentially allow the understanding of the origin of the shallow band at the M-point in FeSe monolayer materials due to correlation effects on Fe-3d states only. The detailed analysis of ARPES detected quasiparticle bands and LDA+DMFT results shows that this shallow band is formed just by the degenerate Fe-3d$_{xz}$ and Fe-3d$_{yz}$ bands renormalized by correlations. Moreover the so called "replica" band observed in ARPES for FeSe/STO can be reasonably understood as the simple LDA renormalized Fe-3d$_{xy}$ band with no reference to interactions with optical phonons

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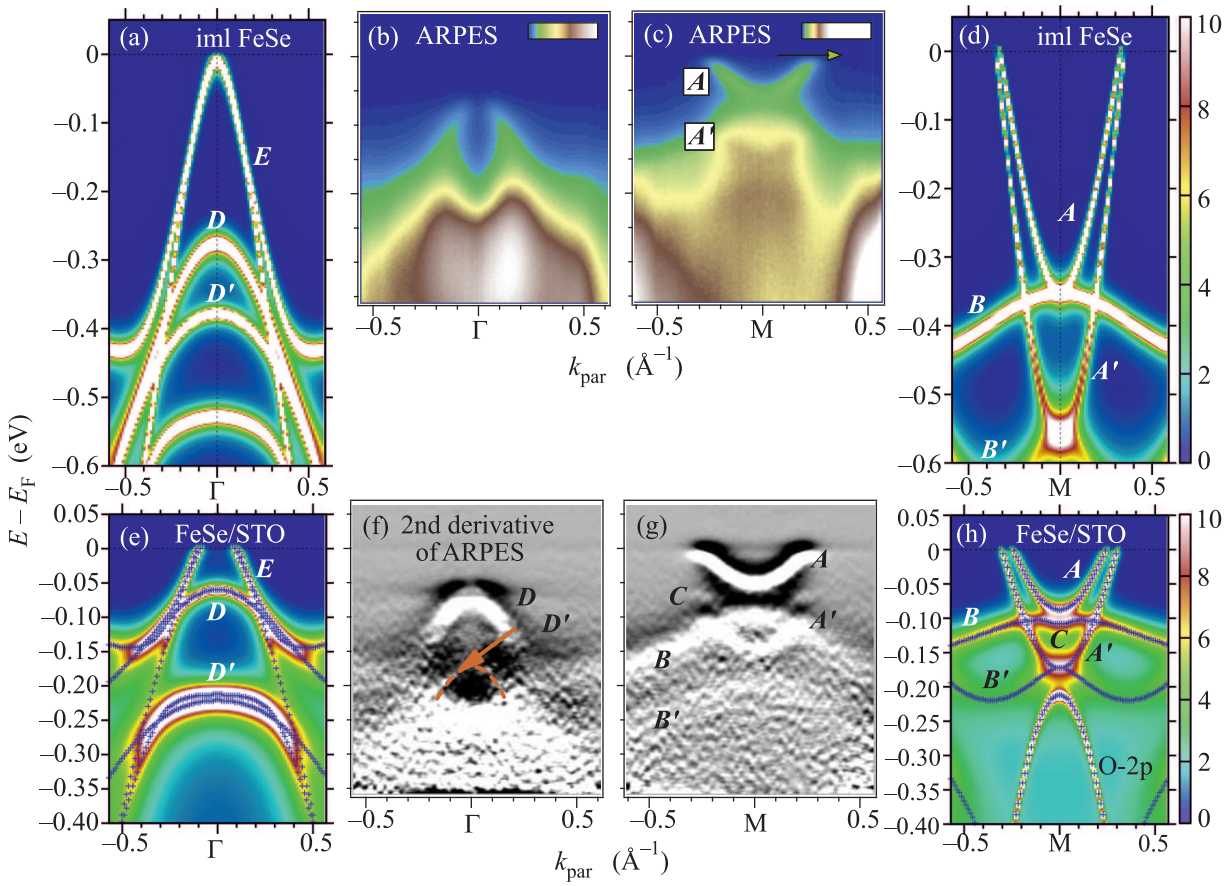

Fig. 1. (Color online) (a), (d) – LDA+DMFT spectral function maps of isolated FeSe monolayer. (b), (c) – Experimental ARPES data around Γ and M points. (f), (g) – Corresponding second derivatives of ARPES data for FeSe/STO [1]. (e), (h) – LDA+DMFT spectral function maps with maxima shown with crosses for FeSe/STO. To mark similar features of experimental and theoretical spectral function maps A, B, C, D, E letters are used. Fermi level is at zero energy

of STO. The influence of STO substrate in our calculations is reduced only to the removal of degeneracy of Fe-3d$_{xz}$ and Fe-3d$_{yz}$ bands in the vicinity of M-point.

In the case of $K_xFe_{2-y}Se_2$ most of ARPES detected bands can also be expressed as correlation renormalized Fe-3d LDA bands.

Unfortunately correlation effects are unable to completely eliminate the hole Fermi surface at the Γ-point, which is not observed in most ARPES experiments on FeSe/STO system. Note, however, that recently a small Fermi surface at the Γ-point was observed in ARPES measurements on FeSe/STO at doping levels, corresponding to the highest values of T_c [10].

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