Electronic structure of FeSe monolayer and $K_{1-x}Fe_{2-y}Se_2$ superconductors: shallow bands and correlations

RUSSIAN ACADEMY OF SCIENCES
URALS DIVISION
Institute of Electrophysics

N.S. Pavlov[1], I.A. Nekrasov[1], M.V. Sadovskii[1,2]

[1]Institute for Electrophysics UB RAS, 620016, Russia, Ekaterinburg, Amundsen str. 106
[2]Institute of Metal Physics UB RAS, 620108, Russia, Ekaterinburg, S. Kovalevskoy str. 18

E-mail: pavlovns@gmail.com

JETP Letters **105**, 370 (2017) arXiv:1702.00949
JETP **126**, 485 (2018) arXiv:1707.05262

Introduction

Some iron chalcogenides superconductors ($K_{1-x}Fe_{2-y}Se_2$, FeSe/$SrTiO_3$, $[Li_{1-x}Fe_xOH]FeSe$) have qualitatively different electronic properties from other iron-based superconductors (e.g. iron pnictides).

Electronic spectra of typical single FeSe layer superconductors FeSe monolayer films on SrTiO3 substrate (FeSe/STO) and $K_xFe_{2-y}Se_2$ obtained from ARPES data reveal several puzzles: what is the origin of shallow and the so called «replica» bands near M-point and why the hole-like Fermi surfaces near Γ-point are absent. While for the iron pnictides and some iron chalcogenides (e.g. bulk FeSe) these hole-like Fermi surface sheets near the Γ-point were clearly observed by ARPES.

The absence of the hole-like Fermi surface sheets near the Γ-point indicates that for FeSe series there is no possibility of nesting between the hole sheets of the Fermi surface near the Γ-point and electronic sheets near the M-point. Thus a spin-fluctuation mechanism of superconducting pairing (assumed for iron pnictides[1]) is not applicable here.

[1]P.J. Hirshfeld, M.M. Korshunov, I.I. Mazin. Rep. Prog. Phys. **74**, 124508 (2011)

Recently in the work[2] was reported ARPES observation of a hidden hole-like band approaching the Fermi level near the Γ-point for the $K_{0.62}Fe_{1.7}Se_2$ system. Also in the work[2] on the basis of the ARPES data analysis there was proposed a presence of a hidden hole-like Fermi surface near the Γ-point. The authors[2] provide some reasons why the Fermi surfaces near the Γ-point previously were not observed due to the geometry of the experiment.

[2]M. Sunagawa et al., J. Phys. Soc. Jpn. **85**, 073704 (2016)

Method and computation details

For *ab anitio* calculations local density approximation (LDA) was employed (LDA well describes the compounds of s and p chemical elements). To describe strongly-correlated electron states (Fe-3d electron states) the Hubbard model was used. The Hubbard model was solved in limit of infinity space dimensional by dynamical mean-field theory (DMFT). For DMFT part of LDA+DMFT[3] calculations we employed the CT-QMC impurity solver (TRIQS[4]). LDA'[5] calculations of KFe_2Se_2 compound were performed using the Linearized Muffin-Tin Orbitals method (LMTO).

[3]G. Kotliar et al. Rev. Mod. Phys. **78**, 865 (2006)

[4]M. Ferrero, O. Parcollet., TRIQS: a Toolbox for Research in Interacting Quantum Systems, http://ipht.cea.fr/triqs; M. Aichhorn et al. Phys. Rev. B **80**, 085101 (2009); L. Boehnke et al. Phys. Rev. B **84**, 075145 (2011)

[5]I.A. Nekrasov, N.S. Pavlov, M.V. Sadovskii, JETP Letters **95**, 581 (2012), arXiv:1204.2361; JETP **116**, 620 (2013), arXiv:1208.4732

The temperature of DMFT calculations: T=1/40 eV (~290 K).

The number of Monte-Carlo sweeps was 10^8.

Parameters of DMFT calcualtion for FeSe/STO:

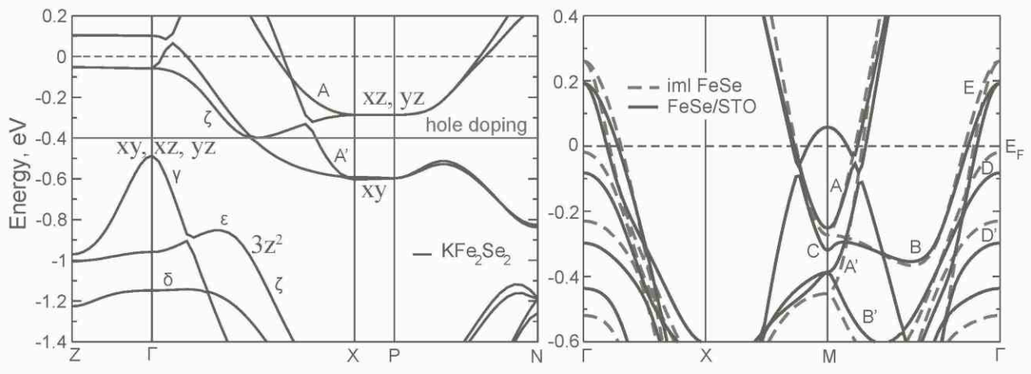
The Coulomb and the Hund interactions: U=5.0 eV, J=0.9 eV. Doping was 0.2 electrons per Fe and Se ions.

Parameters of DMFT calcualtion for $K_{0.62}Fe_{1.7}Se_2$:

The Coulomb and the Hund interactions: U=3.75 eV, J=0.56 eV. Doping was 1.29 holes per Fe and Se ions.

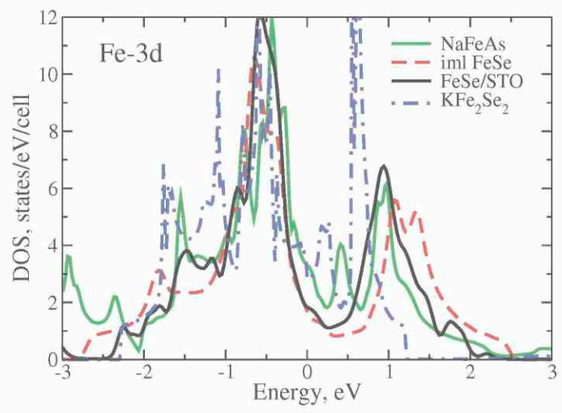
Results of calculations

$K_{0.62}Fe_{1.7}Se_2$: LDA bands FeSe/STO:



Similar bands are marked letters on all panels.

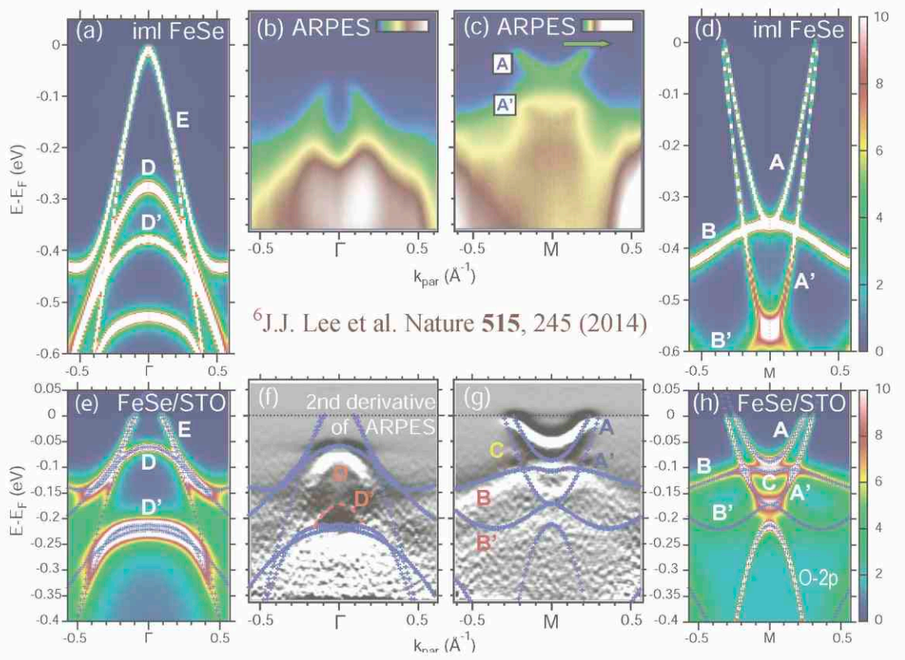
LDA densities of states



NaFeAs W=4.5 eV, iml FeSe W=5.2 eV,
FeSe/STO W=4.3 eV, KFe_2Se_2 W=3.5 eV

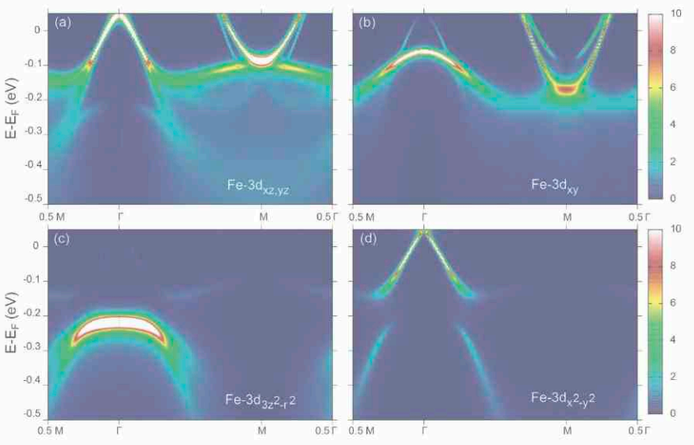
FeSe/STO:

Comparison of the LDA+DMFT spectral function maps with ARPES[6]



[6]J.J. Lee et al. Nature **515**, 245 (2014)

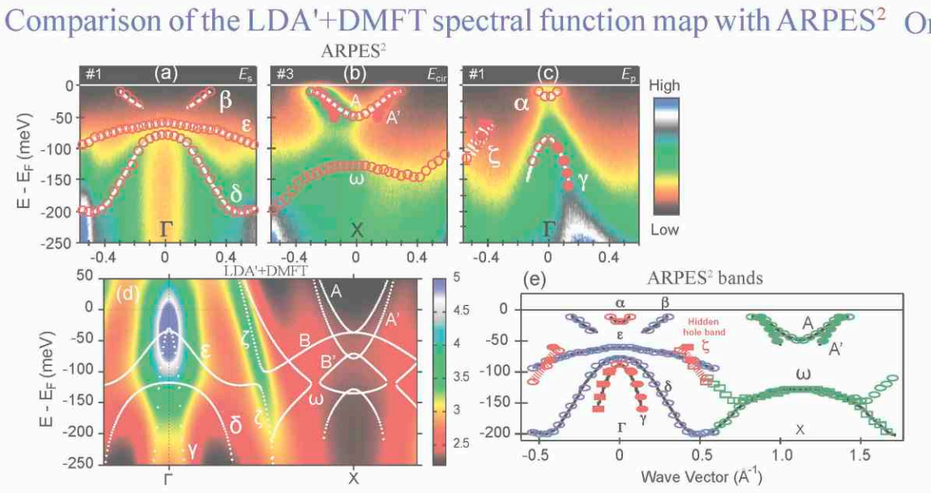
Orbital resolved LDA+DMFT spectral function maps



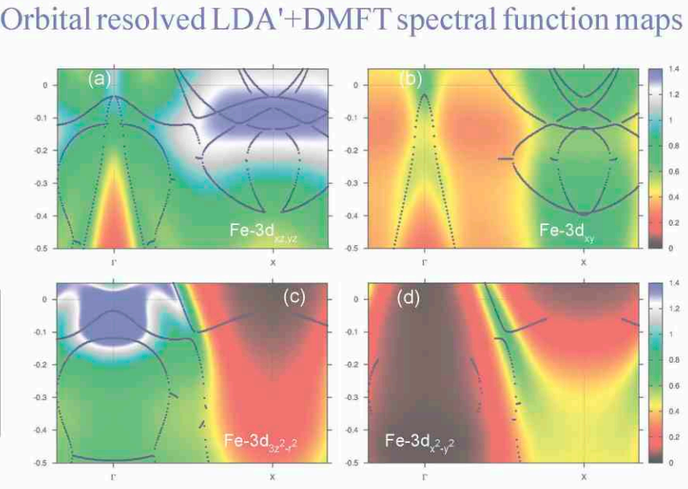
X - LDA+DMFT quasiparticle bands

$K_{0.62}Fe_{1.7}Se_2$:

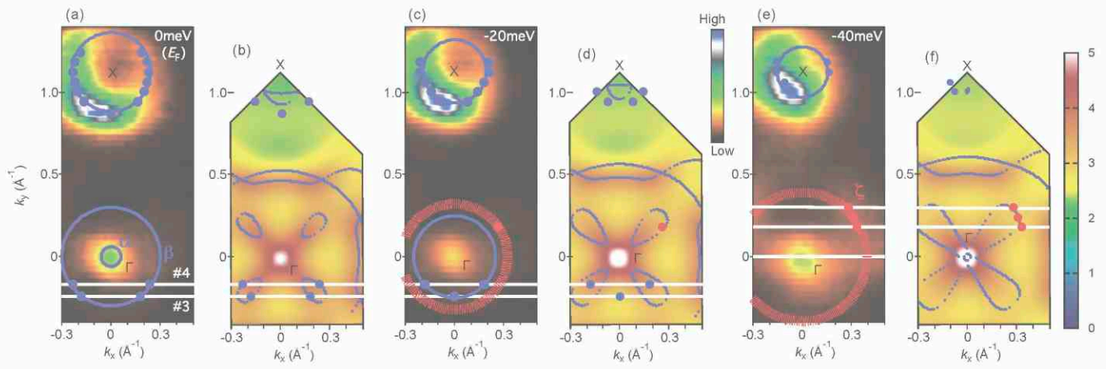
Comparison of the LDA'+DMFT spectral function map with ARPES[2]



Orbital resolved LDA'+DMFT spectral function maps



Comparison of the LDA'+DMFT Fermi surface with ARPES[2]



(a,c,e) - ARPES[2].
(b,d,f) - LDA'+DMFT Fermi surface maps.
The red and blue dots on (b,d,f) are the same points as on (a,c,e).

Conclusion

Our extensive LDA+DMFT calculations show that correlation effects on Fe-3d states can almost quantitatively reproduce rather complicated band structure, which is observed in ARPES, in close vicinity of the Fermi level for FeSe/STO and $K_{0.62}Fe_{1.7}Se_2$.

Rather unusual shallow electron-like bands around the M(X)-point in the Brillouin zone are well reproduced. However, in FeSe/STO correlation effects are apparently insucient to eliminate the hole-like Fermi surfaces around the Γ-point, which are not observed in most ARPES experiments.

It is shown that for FeSe/STO system the LDA calculated Fe-3d_{xy} band, renormalized by electronic correlations within DMFT gives the quasiparticle band almost exactly in the energy region of the experimentally observed "replica" quasiparticle band at the M-point.

For the case of $K_{0.62}Fe_{1.7}Se_2$ most bands observed in ARPES can also be understood as correlation renormalized Fe-3d LDA calculated bands, with overall semi-quantitative agreement with our LDA'+DMFT calculations.

Thus the shallow bands near the M-point are common feature for FeSe-based systems, not just FeSe/STO.

Also it is shown that near the Γ-point the two hole bands cross the Fermi level for $K_{0.62}Fe_{1.7}Se_2$. One band has the Fe-3d_{xy} orbital character, the second - Fe-3$d_{yz, xz}$. There are the hidden hole-like Fermi surfaces near the Γ-point in $K_{0.62}Fe_{1.7}Se_2$. Consequently, this compound is similar to FeAs-based compounds, and suggests the possible existence of a similar superconductivity mechanism.

This work was done under the State contract (FASO) No. 0389-2014-0001 and supported in part by RFBR grant No. 17-02-00015 and the Program of Fundamental Research of the RAS Presidium «Fundamental problems of high - temperature superconductivity».

Thank you for attention!