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## ELECTRONIC STRUCTURE AND PROPERTIES

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# Anomalous Downshift of Electronic Bands in Fe(Se, Te) in Superconducting State

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In this article we are provided the temperature dependent angle-resolved photoemission spectroscopy (ARPES) study of different iron-based superconductors (FeSe, Fe(Se, Te), Ba(Co, Fe)As) in the vicinity of the superconducting transition. The existence of a strong downshift of the bands in the centre of the Brillouin zone (BZ) with temperature decrease is established for Fe(Se, Te). The value of such a shift for temperatures 4 K and 20 K is approximately 5 meV. Such changes are not observed for the $d_{yz}$ band of Ba(Co, Fe)$_2$As$_2$ and for the $d_{xz}$ band of FeSe. The observed strong dependence is likely to be the result of an interplay between the superconducting state and the mechanism that shifts bands in the temperature range from 20 to 300 K.

**Key words:** iron-based superconductors, ARPES, FeSe, electronic band structure, iron pnictides, iron chalcogenides.

У статті наведено результати ARPES дослідження різних залізовмісних надпровідників (FeSe, Fe(Se, Te), Ba(Co, Fe)As) для температур поблизу температури надпровідного переходу. Встановлено існування сильного зсуву зон у центрі зони Бріллюена у напрямку підвищення енергії зв'язку для Fe(Se, Te). Величина цього зсуву склала приблизно 5 меВ для темпе-

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ратур 20 К та 4 К. Такий зсув не спостерігався для $d_{yz}$ зони Ba(Co, Fe)$_2$As$_2$ та $d_{xz}$ зони FeSe. Сильна температурна залежність, що спостерігається, може бути результатом взаємодії між надпровідним станом та механізмом, що відповідає за зсув зон у температурному діапазоні 20–300 К.

**Ключові слова:** залізовмісні надпровідники, ARPES, FeSe, зонна структура, феропніктиди, фероселеніди.

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## 1. INTRODUCTION

FeSe is one of the most interesting compounds among iron based superconductors, which displays a variety of complex and competing electronic phases. The superconductivity in FeSe seems to compete with rather stable electronic 'nematic' phase, the transition to which is not followed immediately by the transition to the antiferromagnetic phase like in all other iron based superconductors [1–3]. The electronic nature of the nematic transition in FeSe has been demonstrated by numerous Raman measurements [4]. However, the electronic structure of FeSe also attracts a great attention due to the strong correlation between the critical temperature and the Fermi surface topology [2].

An additional factor stimulating interest to the FeSe studies is the ability of FeSe to exhibit antiferromagnetic properties [5, 6]. Considering the antiferromagnetic spintronics [5] is now one of the emergent fields of the physics of magnetism and applied physics, the study of FeSe can be relevant for the development of various spintronic systems, including neuromorphic systems based on artificial 'neurons' similar to the 'traditional' antiferromagnetic 'neurons' [6, 7].

One of the characteristic features of FeSe is the strong temperature dependence of its electronic band structure that has been revealed in recent papers. Despite some discrepancies for interpretation of the temperature-dependent ARPES data for the BZ centre (Z-point), it is more likely that all bands in the vicinity of the Fermi-level move downwards in energy with temperature increase [8–10]. Also it should be mentioned that, taking into account the evolution of the electronic structure in the corners of the Brillouin zone (A-point), the observed shifts should lead to a change of the charge carrier concentration in the system. Despite some suggestions [10], the physical mechanism for such shifts remains an open issue.

In this paper, we reveal temperature induced shifts of the band structure in the centre of the Brillouin zone (BZ) of Fe(Se, Te) in vicinity to superconducting transition. It has been established that both the $d_{xz}$ and $d_{yz}$ bands shift downwards in energy as the compound undergoes superconducting transition. For the temperatures 4 K and 20 K, the value of such a shift is approximately 5 meV. Such shifts have not

been observed for $d_{yz}$ band of $Ba(Co, Fe)_2As_2$ and for $d_{xz}$ band for FeSe. So we conclude that this shift is the characteristic feature of Fe(Se, Te) and suppose a change of direction of the shift of the bands with temperature increase. This change may be a result of a superconductivity induced suppression of the physical mechanism that shifts the bands in the temperature range from 20 to 300 K.

## 2. EXPERIMENTAL DETAILS

Angle-resolved photoemission spectroscopy (ARPES) enables direct observation of the Fermi surface and underlying electronic structure of crystals, which are the basic concepts necessary to describe all the electronic properties of solids and to reveal the nature of key electronic interactions involved. More details about the method can be found in our review [11] or in the most recent review [3].

The ARPES spectra from Z point (the Brillouin zone centre) of $Fe_{1.05}Se_{0.84}Te_{0.16}$ for the temperatures 4 K and 20 K have been obtained on CASIOPEE beamline of synchrotron Soleil using horizontally polarized radiation with energy 21 eV.

The ARPES spectra from Z point of FeSe in the range from 1.55 K to 15.1 K and of $Ba(Co, Fe)_2As_2$ in the range from 1.1 K to 26 K have been obtained on the '1–3' beamline of the BESSY synchrotron using 23 eV (FeSe) and 50 eV ($Ba(Co, Fe)_2As$) photons.

The $Fe_{1.05}Se_{0.84}Te_{0.16}$ crystal used here is from the same batch as the crystal that is studied in [10].

## 3. RESULTS AND DISCUSSION

To investigate the temperature induced changes of the band structure, a two-dimensional curvature method has been used. Besides good visual representation of ARPES spectra, the method is more accurate in determination of the renormalized band dispersion than both the distribution curves fitting and the momentum distribution curves fitting procedures [12, 13]. Figure 1 shows the results of processing of ARPES spectra of $Ba(Fe, Co)_2As_2$ obtained for temperatures 1.1 K and 26 K with the curvature method. In this case, on processed ARPES spectra the $d_{xz}$-band can be seen.

Figure 2 shows the results of processing of the spectra of FeSe obtained for 1.55 K and 15.1 K with the curvature method. In this case, on processed ARPES spectra the $d_{yz}$-band can be seen.

The shift of energy distribution curve (EDC) leading edge has been used to determine that FeSe undergoes superconducting transition and to estimate the value of the superconducting gap [14, 15]. The leading edge position is the position of highest absolute value of the EDC's

derivate, so to determine leading edge the region near the EDC derivative minimum has been fitted to Gauss profile. As a rule, a leading edge gap is approximately two times smaller than the real gap size [14].

The determined leading edge position is presented in Fig. 3. It reveals the existence of the superconducting transition with the gap size approximately 3 meV. As one can see from Fig. 1 and Fig. 2, neither

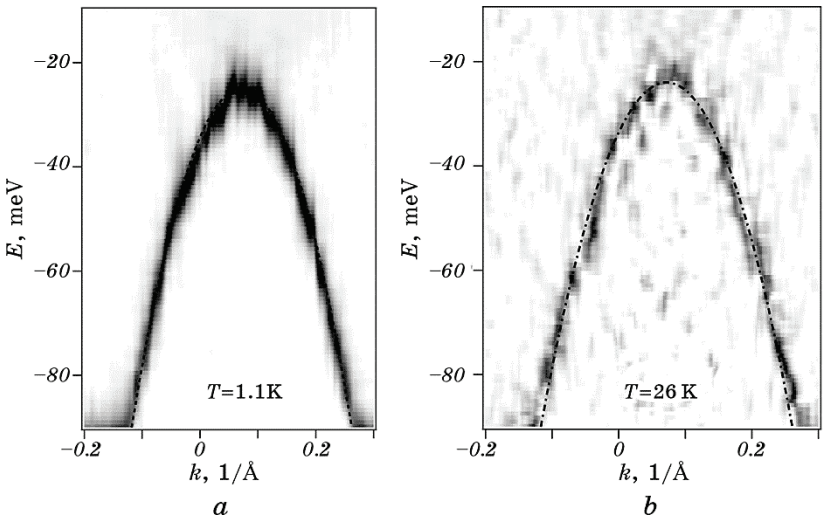


**Fig. 1.** The results of the ARPES spectra processing with the curvature method for $Ba(Fe, Co)_2As_2$ for the temperatures 1.1 K and 26 K.

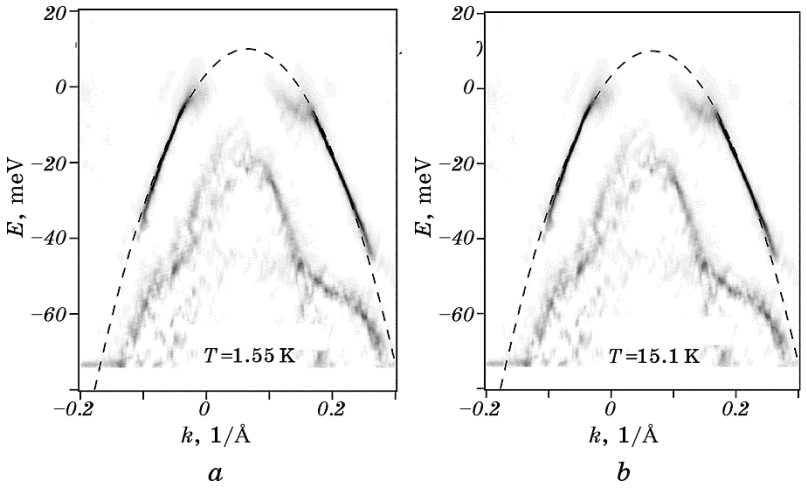


**Fig. 2.** The results of the ARPES spectra processing with the curvature method for FeSe for the temperatures 1.55 K and 15.1 K.

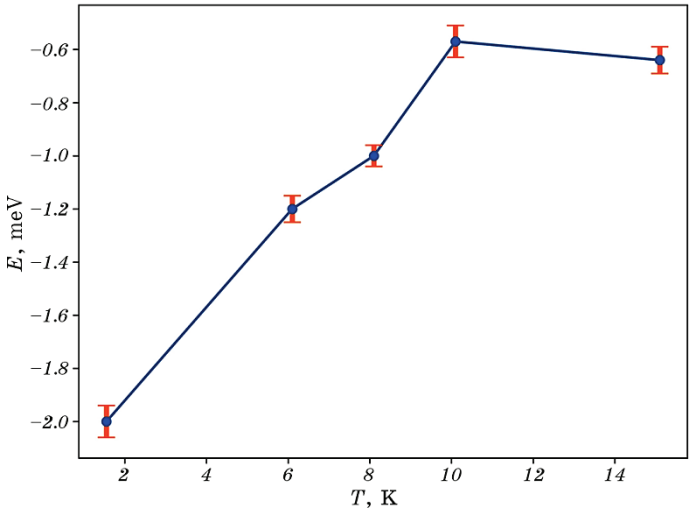


**Fig. 3.** The EDC leading edge position obtained from ARPES spectra of FeSe for 1.55, 6.1, 8.1, 10.1, and 15.1 K.

the $d_{xz}$-band for $Ba(Fe, Co)_2As_2$ nor the $d_{yz}$-band for FeSe are shifting.

Figure 4 shows the results of the processing of $Fe_{1.05}Se_{0.84}Te_{0.16}$ spectra obtained for 4 K and 20 K with the curvature method. In this case, the $d_{yz}$ and $d_{xz}$ bands can be seen on the spectra. Figure 4 reveals completely different case for $Fe_{1.05}Se_{0.84}Te_{0.16}$—both the bands in the centre

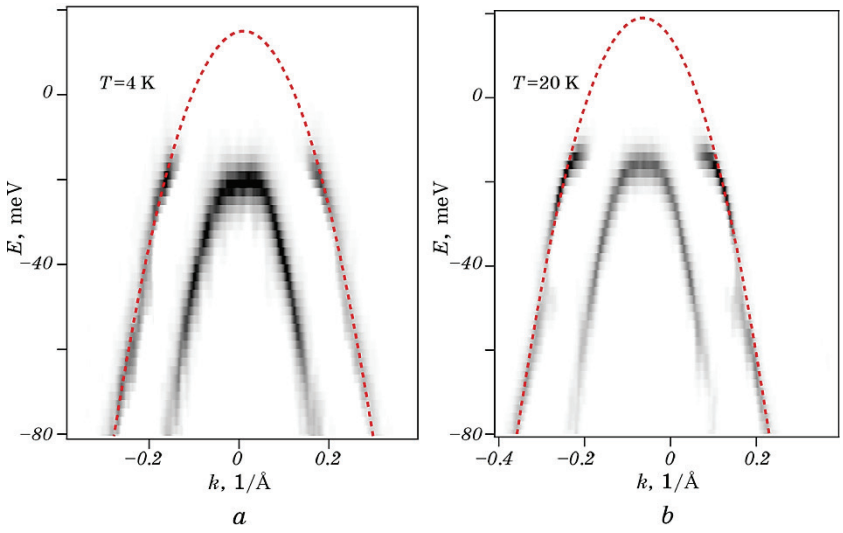


**Fig. 4.** The results of the ARPES spectra processing with the curvature method for $Fe_{1.05}Se_{0.84}Te_{0.16}$ for the temperatures 4 K and 20 K.

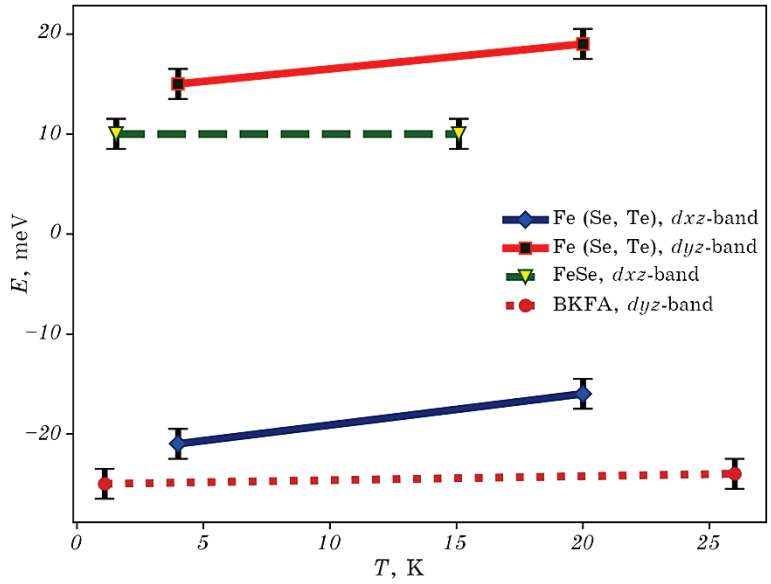


**Fig. 5.** The positions of different bands for different iron-based compounds for temperatures higher and lower than the temperature of superconducting transition. ($Fe_{1.05}Se_{0.84}Te_{0.16}$—solid line, $Ba(Fe, Co)_2As_2$—dotted line, FeSe—dashed line).

of the Brillouin zone move downwards in energies when $Fe_{1.05}Se_{0.84}Te_{0.16}$ undergoes the superconducting transition. The value of this shift is approximately 5 meV and its direction is opposite to the direction obtained in [9, 10] for temperature range 20–300K. Therefore, we can conclude that superconducting transition suppresses the mechanism that changes the charge carrier concentration (Fig. 5).

## 4. SUMMARY

We have performed the temperature-dependent ARPES study of the high quality single crystals of $Fe_{1.05}Se_{0.84}Te_{0.16}$, $Ba(Co, Fe)_2As_2$, and FeSe in the vicinity of the superconducting transition. The strong downshift of both the hole-like bands for $Fe_{1.05}Se_{0.84}Te_{0.16}$ with decreasing temperature has been revealed. For the $Ba(Co, Fe)_2As_2$ and FeSe crystals, we have not observed any essential shift of the bands for the temperatures below the superconducting transition. Based on the observed changes we conclude that the superconducting transition tends to compensate the physical mechanism that is responsible for the strong temperature-induced changes of the band structure in the 20–300 K temperature range.

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