

Temperature induced shift of electronic band structure in Fe(Se,Te)

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FeSe, the simplest iron-based superconductor, reveals a variety of puzzling properties and features that could hold a key for the pairing mechanism in this family of superconductors. In particular, its complex electronic band structure differs essentially from the DFT calculated one in a special way called the “red-blue shift” and, in addition, drifts anomalously with temperature. Here we study this band structure evolution in Fe(Se,Te) crystals and reveal essential downdrift of all the hole-like bands with increasing temperature, which is opposite to the “red-blue shift” expectation. We show that this drift cannot be described by temperature-dependent contribution to quasiparticle self-energy within the Fermi-liquid concept but could result in charge redistribution between the bulk and topological surface states. If such a scenario is confirmed, one can tune the topologically non-trivial bands near the Fermi level with temperature, potentially allowing temperature-induced crossover between different Fermi surface topologies.

Keywords: electronic band structure, Fermi level, pnictides, chalcogenides.

1. Introduction

The iron-based pnictides and chalcogenides form a new class of superconductors that has attracted a tremendous interest due to revived hope to find finally a key to understand the mechanism of high-temperature superconductivity [1–3]. FeSe is the simplest compound in this class and has therefore been considered as a perfect object for theoretical and experimental investigations [4–7].

In reality, it has been found that FeSe-based compounds do not behave as simple superconductors but reveal a number of very surprising properties: The critical temperature of FeSe single crystals can be highly increased by applying pressure [8], by intercalation [9–11], or in the single layer FeSe film on STO substrate [12–14]. At the same time, the superconductivity in FeSe seems to compete with rather stable electronic “nematic” phase [15,16], the transition to which is not followed immediately by the transition to the antiferromagnetic phase as in all other iron based superconductors [3,6]. The effect of the nematic transition on the electronic band structure is strong enough to relate its origin with intrinsic electronic instability due to some anomalous electron-electron interaction [17]. The observed systematic differences of the experimental electronic band structure from the DFT calculation results, called the “red-blue shift” [6,18], can be another manifestation of that interaction.

Then, it is probably not so strange, that the band structure of all FeSe-based compounds changes strongly with temperature also well above the nematic transition [19,20]. These changes, however, are not well-investigated yet [21]. There are several temperature-dependent angle resolved photoemission spectroscopy (ARPES) studies of FeSe in the corner and in the center of the Brillouin zone (BZ) [19,20]. Despite an agreement in interpretation of ARPES data obtained in the BZ corner (*A*-point), there are some discrepancies for the BZ center (*Z*-point). In [20], it was established that d_{xz} and d_{yz} -bands move downwards in energy with temperature increase, whereas in [19], the direction of the evolution is opposite.

So, while an intimate relation between electronic band structure and critical temperature of almost all the iron-based superconductors has been revealed [3,6,21,22], the electronic structure of the simplest compound from this family is not well understood. There is no consensus even on direction of the band structure evolution with temperature, not to say about its driving force [21]. Finally, an additional value for the importance of studying the band structure of the FeSe based compounds comes from recent suggestion about existence of the intrinsic topological superconducting states in FeSe_{0.5}Te_{0.5} crystals [23], which do not differ much from the pure FeSe [6]. If confirmed, it opens a playground for engineering different topological states in different iron based superconductors [24] that will

be indispensable for future spintronic applications. And temperature will be crucial parameter, taking into account the discussed here effects.

In this paper we study the temperature evolution of the band structure in Fe(Se,Te) single crystals with ARPES [25,26]. We observe essential downshift of all the bands in the BZ center of Fe(Se,Te) with increasing temperature, that is opposite to the “red-blue shift” expectation [6,21] and to recent observation [19] but is consistent with another experiment [20] for the pure FeSe crystals. We show that this shift cannot be described by temperature dependent contribution to quasiparticle self-energy within the Fermi-liquid concept but could be a result of intrinsic inhomogeneity general for FeSe-based superconductors.

2. Experimental details

ARPES spectra of the Z-point of the BZ have been obtained on CASIOPEE beamline of synchrotron Soleil using radiation with linear vertical (LV) and linear horizontal (LH) polarization with energy 21 eV, for temperature range between 20 K and 250 K. The crystals $\text{Fe}_{1.05}\text{Se}_{0.84}\text{Te}_{0.16}$ have been grown in evacuated quartz ampoules using the $\text{AlCl}_3\text{-KCl-NaCl}$ flux technique with a constant temperature gradient (500 °C temperature of the hot end, 430 °C temperature of the cold end, $\text{Fe}_{1.3}\text{Se}_{0.8}\text{Te}_{0.2}$ composition of the start load, 6 weeks) [27]. The chemical composition of the Fe(Se,Te) crystals was determined using a Tescan Vega II XMU scanning electron microscope equipped with

an INCA Energy 450 energy-dispersive spectrometer (20 kV accelerating voltage).

3. Results

Different bands can be observed for different photon polarizations, due to the matrix elements effect [25,26]. For the central cut of BZ of FeSe for the LV polarized radiation the Fe d_{xz} band is mainly seen, while for the LH polarized light—all the Fe d_{xz} , d_{yz} and Se p_z band become more visible. 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 the energy distribution curves fitting procedures [28]. Figure 1 shows ARPES spectra obtained by the LV polarized radiation for temperatures 20 K (Fig. 1(a)), 100 K (b), 160 K (c), 220 K (d), and the results of processing data with the curvature method (e)–(h). One can see, that the d_{xz} band moves downwards in energy monotonically and the dependence of band position on temperature is linear in a wide temperature range. The estimated value of this temperature-induced shift is approximately 1.3 meV per 10 K.

In Fig. 2 the ARPES spectra obtained using the LH polarized radiation for temperatures 20 K (a), 100 K (b), 160 K (c) are shown. The results of their processing with two-dimensional curvature method are given respectively in (d)–(f). We see that the positions of d_{xz} band in spectra

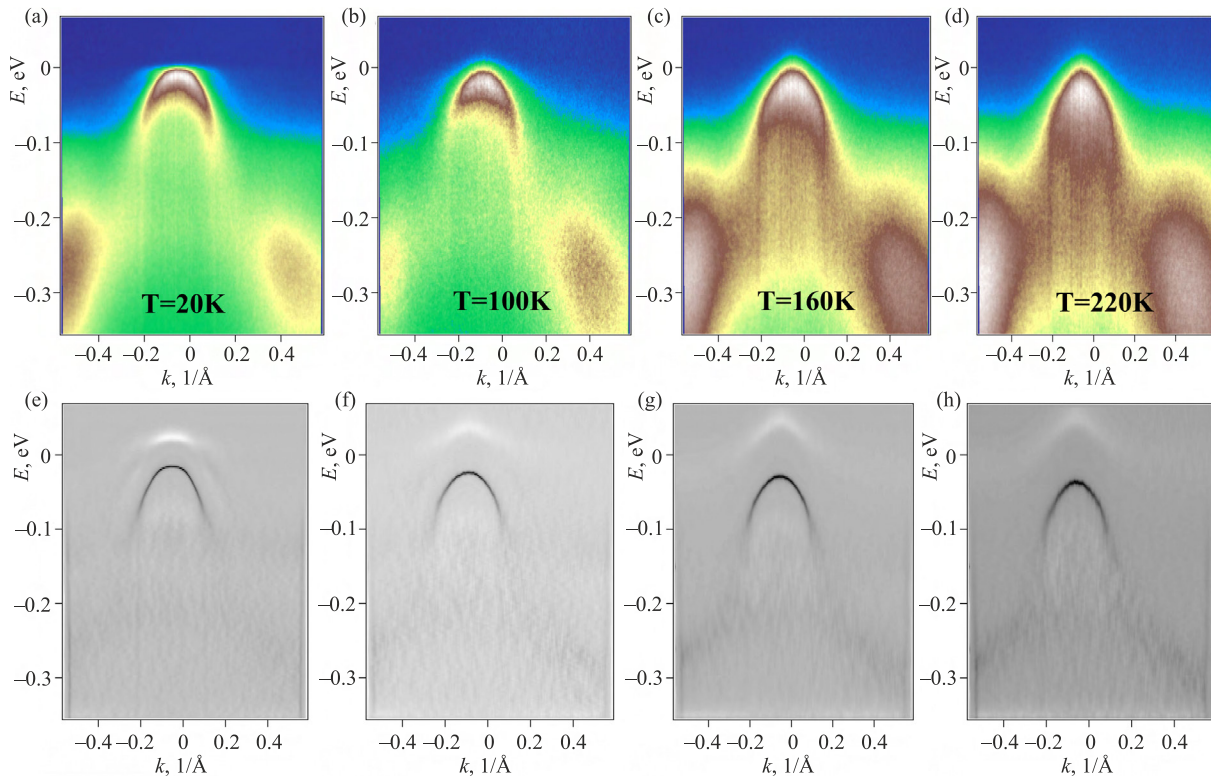


Fig. 1. (Color online) ARPES spectra of $\text{Fe}_{1.05}\text{Se}_{0.84}\text{Te}_{0.16}$ from the center of the Brillouin zone (Z-point) obtained with the vertically polarized 21 eV photons at T , K: 20 (a), 100 (b), 160 (c), and 220 (d). The same spectra processed with the curvature method (e)–(h).

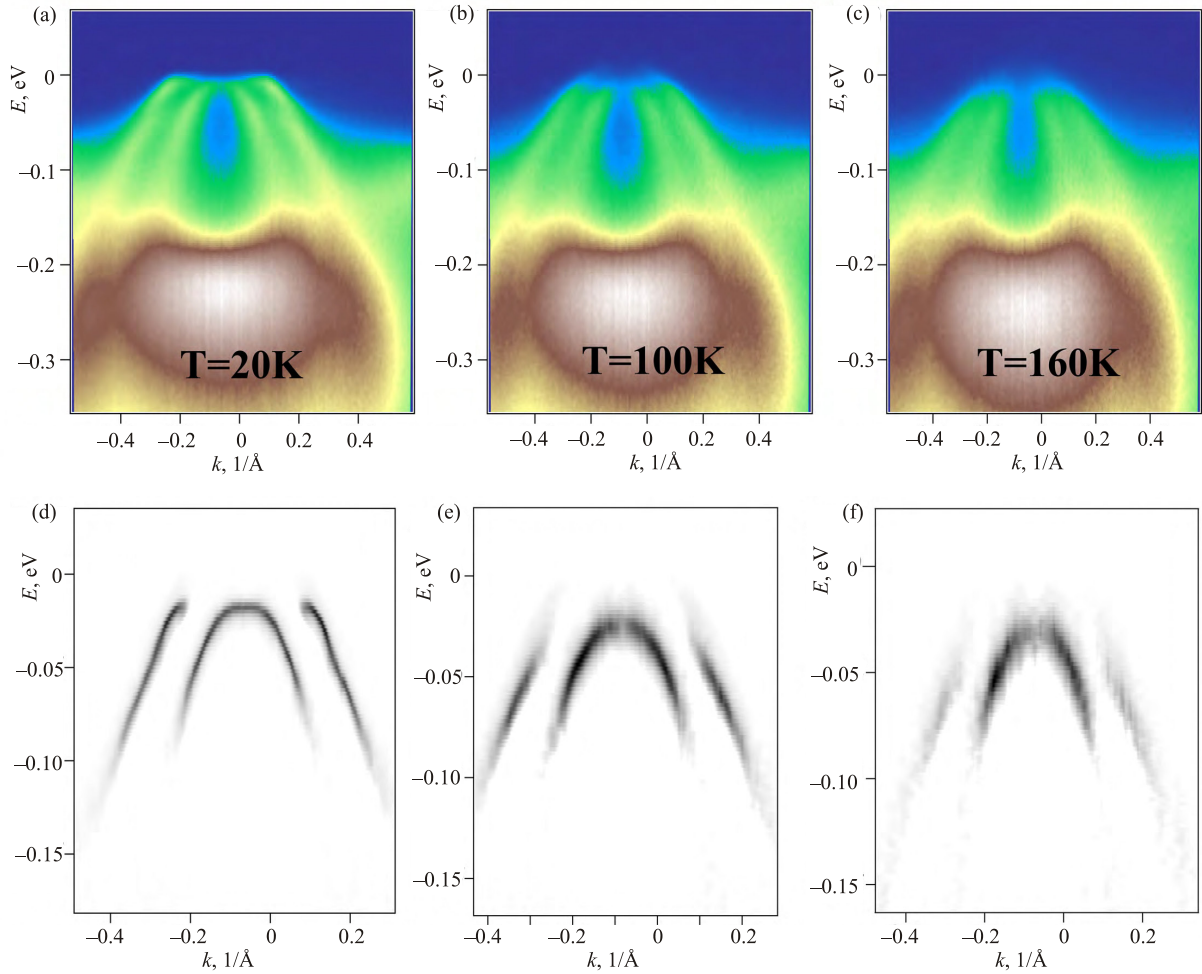


Fig. 2. (Color online) ARPES spectra of $\text{Fe}_{1.05}\text{Se}_{0.84}\text{Te}_{0.16}$ from the center of the Brillouin zone (Z-point) obtained with the horizontally polarized 21 eV photons at T , K: 20 (a), 100 (b), and 160 (c). The same spectra processed with the curvature method (d)–(f).

obtained with orthogonal polarizations coincide. The d_{xz} and d_{yz} bands move to higher binding energies with the same speed in a wide temperature range 20–160 K. It is important to mention, that the shift of the d_{yz} -band reduces the area of the hole-like Fermi surface in the center of BZ. We summarize the obtained temperature induced shifts of the band structure for ARPES spectra obtained with the LV and the LH polarized radiation in Fig. 3.

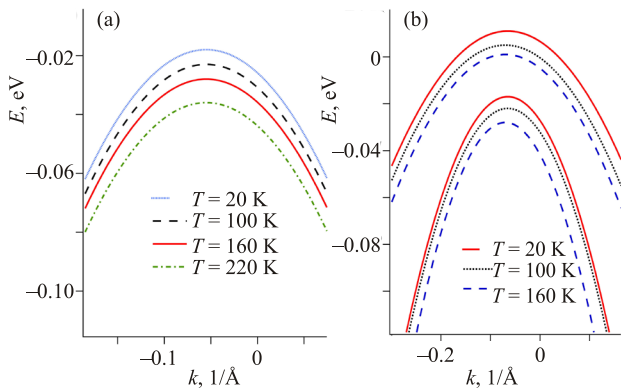


Fig. 3. (Color online) Electronic dispersion of d_{xz} and d_{yz} bands obtained from spectra with LV (a) and LH (b) polarized radiation.

The curvature method can hardly be used to determine the position of the p_z band due to low intensity of this band. Also the low Fermi velocity makes MDC analysis inapplicable [26]. To estimate the position of the Se p_z band for different temperatures, the energy distribution curves (EDC) integrated in the $[-0.09 \text{ 1/Å}, 0.09 \text{ 1/Å}]$ momentum window have been analyzed and the positions of their maxima for different temperatures have been determined. The data show that the band moves in the same direction as the d_{xz} and d_{yz} bands. The estimated maximal and minimal values of temperature induced shift for this band are 2.1 meV and 0.8 meV per 10 K respectively.

So, one can conclude that all the Fe d_{xz} , d_{yz} , and Se p_z bands in the center of the Brillouin zone of FeSe doped with Te move downwards in energy with increasing temperature with similar speed (see Fig. 4).

4. Discussion

To describe the changes of the d_{xz} band with temperature we try to analyze the temperature dependence within the Fermi liquid model. The imaginary part of the self-energy can be expressed as $\Sigma''(\omega, T) = \alpha\omega^2 + \beta(k_B T)^2 + \text{Imp}$, where constant parameter Imp is added to take into ac-

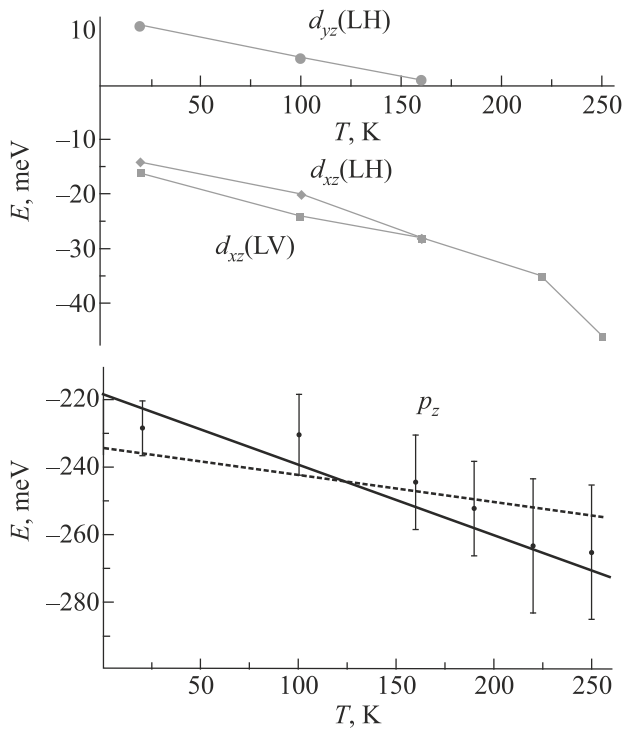


Fig. 4. Position of the tops of the d_{xz} , d_{yz} bands derived from the spectra obtained with the LV and the LH polarized radiation with two-dimensional curvature method and the position of p_z band derived from EDC analysis with error-bars for different temperatures.

count the scattering on impurities. The real part of the self-energy is expected to depend on temperature and energy linearly, so $\Sigma'(\omega, T) = -\lambda\omega - \gamma k_B T$ [29]. The bare electron dispersion is approximated by simple parabola $\varepsilon(k) = bk^2 + l$.

Disregarding the matrix elements effect the photoelectric intensity will be $I(k, \omega) = A(k, \omega)f(\omega)$, where $f(\omega)$ is the Fermi function. Value of $\lambda = 3.35$ was taken from [6]. Another values of parameters, that give the best approximation of experimentally obtained data are $\alpha = 35 \text{ eV}^{-1}$; $\beta = 10 \text{ eV}^{-1}$; $\gamma = 5.1$; $\text{Imp} = 0.08 \text{ eV}$; $b = -12.1 \text{ eV}\cdot\text{\AA}^2$; $l = -0.06 \text{ eV}$.

In Fig. 5 the results of processing of modeled (a) and experimentally (b) obtained ARPES spectra with the two-dimensional curvature method are given. As one can see, both dispersions behave similarly in a wide temperature range. In Fig. 5(c), (d) the same data but are shown in quadratic momentum scale in order to check possible influence of the Fermi function of the band shift and shape. One can see that all the bands in quadratic momentum scale are pretty linear that means they can be very well described by quadratic dependence and the influence of the Fermi function can be neglected.

It is natural to expect that the ratios γ/β and λ/α should be comparable, but in our case $\gamma/\beta \approx 0.5 \gg \lambda/\alpha \approx 0.1$, so the temperature dependence of the real part of the self-energy is about 5 times stronger than one would expect within the Fermi liquid model.

With the results of evolution of the electronic structure in the corners of the Brillouin zone (A -point) [19,20], the observed shifts should lead to a change of charge carrier concentration in the system. It is about $10 \text{ meV} / 100 \text{ K}$, is similar to shift observed for the FeSe crystal [20], and that is too large [20] to be explained as a consequence of chemical potential shift due to its proximity to the edges of the bands [30,31]. So, the observed shifts contradict to the Luttinger theorem [32] and it is unlikely that they can result from strong temperature dependence of the quasiparticle self-energy.

One can think of different scenarios why the band structure occupation seen by ARPES is changing with temperature and where the extra electrons appear from. It can be redistribution of charge carriers between different phases since it is known that in these compounds the superconducting phase is often inhomogeneous [33] and coexists with another phases, e.g. with the hexagonal insulating phase [27,34,35]. Alternatively, it can be temperature induced localization of itinerant electrons. Finally, it can be charge redistribution between bulk and surface electronic states, that can be clearly seen in topological insulators [36,37].

The later scenario is resonating with recent discovery of topological states in iron based superconductors [23,24] and, in the first place, in Fe(Se,Te) [23,38]. Band calculations have predicted that FeSe_{0.5}Te_{0.5} has a non-trivial topological invariance and hosts topological surface states near the Fermi level [38]. Then recent ARPES experiments have observed in FeSe_{0.55}Te_{0.45} the Dirac-cone type surface states and their spin-helical texture [23]. In further studies [24], it has been found that different topological states should appear in many iron based superconductors, and some experimental evidences are already obtained. One can think about it as temperature dependent band bending [39], but taking into account very small surface-bulk inter-band scattering in topological insulators [40], one may expect much stronger effect, while the reported proximity of the Dirac point to E_F suggests that temperature can be a parameter that allows fine tuning between different topological states.

5. Summary

We have performed a temperature-dependent ARPES study of Fe(Se,Te) in the wide temperature range (from 20 to 250 K) and have revealed the strong temperature drift of all hole-like bands. We show that such drift cannot be explained in terms of strong temperature dependence of quasiparticle self-energy but, most probably, could result in charge redistribution between the bulk and surface states, which now considered to be topological in these compounds. If their non-trivial topological nature is confirmed, one get unique possibility to drive the system between different topological states with temperature or gat-

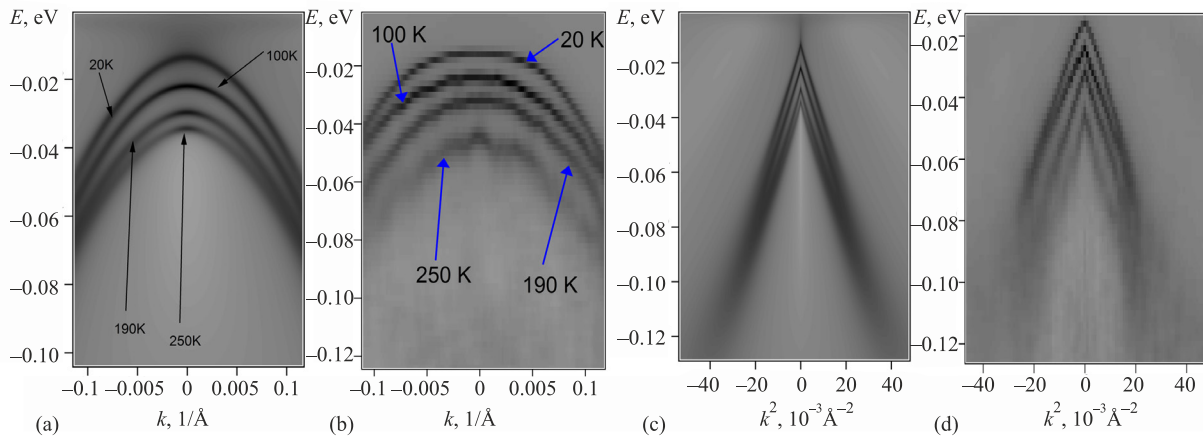


Fig. 5. Electronic dispersion of the d_{xz} band obtained by the two-dimensional curvature method from the modeled (a) and the experimentally obtained (b) spectra. The same spectra but with quadratic momentum scale (c), (d).

ing. This makes the iron based superconductors extremely interesting for possible spintronic applications.

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Температурний зсув електронної зонної структури у Fe(Se,Te)

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FeSe, найпростіший надпровідник на основі заліза, виявляє безліч загадкових властивостей та особливостей, які, можливо, містять ключ до механізму електронного спарювання в цьому сімействі надпровідників. Зокрема, складна електронна зонна структура FeSe істотно та особливим чином відрізняється від розрахованої методами DFT (так званий «червоно-синій зсув») та, крім того, аномально дрейфує з температурою. Досліджено температурну еволюцію зонної

структури у кристалах Fe(Se,Te) та виявлено істотне зниження енергії всіх діркових зон зі збільшенням температури, що суперечить очікуванням моделі «червоно-синього зсуву». Показано, що цей дрейф не може бути описано температурно-залежним внеском у квазічастинкову власну енергію у рамках концепції фермі-рідини, але може бути результатом перерозподілу заряду між об'ємними та топологічними поверхневими станами. Якщо такий сценарій буде підтверджено, можна буде за допомогою зміни температури керувати положенням топологічно-нетривіальних зон поблизу рівня Фермі, що потенційно дозволить реалізувати індукований температурою перехід між топологічно різними поверхнями Фермі.

Ключові слова: електронна зонна структура, рівень Фермі, пніктиди, халькогеніди.

Температурный сдвиг электронной зонной структуры в Fe(Se,Te)

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FeSe, самый простой сверхпроводник на основе железа, обнаруживает множество загадочных свойств и особенно-стей, которые, возможно, содержат ключ к механизму электронного спаривания в этом семействе сверхпроводников. В частности, сложная электронная зонная структура FeSe существенно и особым образом отличается от рассчитанной методами DFT (так называемый «красно-синий сдвиг») и, кроме того, аномально дрейфует с температурой. Исследована температурная эволюция зонной структуры в кристаллах Fe(Se,Te) и обнаружено существенное снижение энергии всех дырочных зон с увеличением температуры, что противоречит ожиданиям модели «красно-синего сдвига». Показано, что этот дрейф не может быть описан температурно-зависимым вкладом в квазичастичную собственную энергию в рамках концепции ферми-жидкости, но может быть результатом перераспределения заряда между объемными и топологическими поверхностными состояниями. Если такой сценарий будет подтвержден, можно будет с помощью изменения температуры управлять положением топологически нетривіальных зон вблизи уровня Ферми, что потенциально позволит реализовать индуцированный температурой переход между топологически различными поверхностями Ферми.

Ключевые слова: электронная зонная структура, уровень Ферми, пніктиды, халькогеніди.