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PRESSURE EFFECT ON ELECTRONIC STRUCTURE AND MAGNETIC PROPERTIES OF IRON-BASED HIGH T_C SUPERCONDUCTORS

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Pressure effects on electronic structure and magnetic properties of iron-based superconductors $FeSe_{1-x}Te_x$ ($x \simeq 0, 0.5$ and 1.0) and $LaFeAsO$ are investigated. The superconducting transition was observed at $T_C \simeq 8, 13.6\text{--}14.2,$ and 26 K in $FeSe_{0.963}, FeSe_{0.5}Te_{0.5},$ and $LaFeAsO_{0.85}F_{0.1},$ respectively. The intrinsic magnetic susceptibility χ in the series of $FeSe_{0.963}, FeSe_{0.5}Te_{0.5}$ and $FeTe$ is found to increase gradually approximately 10 times as much with Te content. A kink in the low-field dependence of $\chi(T)$ was detected at $T_M \simeq 135$ K for $LaFeAsO_{0.85}F_{0.1}.$ The electronic structures and paramagnetic susceptibilities of the studied compounds are calculated ab initio in external magnetic field as a function of atomic volume and structural parameter $Z,$ which specifies the relative height of chalcogen atoms above iron plane. The calculated field-induced magnetic moments and their volume derivatives indicate that these systems are in a close proximity to a quantum critical point. For $FeSe$ and $FeTe$ the calculated paramagnetic susceptibilities reveal a large magnetovolume effect and a drastic sensitivity to parameter $Z.$

Keywords: FeAs superconductors, FeSe(Te), pressure effect, magnetization, electronic structure

Following the discovery of the iron-pnictide high T_C superconductors (SCs) [1], a search for the new SCs extended to a variety of iron-based layered compounds like $RFeAs$ («111», $R =$ rare earth metal), AFe_2Se_2 («122», $A =$ divalent alkaline earth metal), $BFeSe$ («111», $B =$ alkali metal), and simple $FeSe(Te)$ materials («11»), which exhibited SC with transition temperatures T_C in the range of

8–55 K [2–5]. Among iron-based SCs, $\text{FeSe}_{1-x}\text{Te}_x$ chalcogenides are distinguished by their structural simplicity. Though SC with medium transition temperatures about $T_C \simeq 8$ K was observed for Se deficient FeSe compounds, the partial replacing of Se with Te has provided $T_C \simeq 15$ K at about 50% Te substitution [6]. Furthermore, the substantial enhancement of T_C was observed in FeSe under high pressures, yielding the SC transition temperatures as high as $T_C \simeq 27$ K [7], 34 K [8], 35 K [9], and 37 K [10]. Large pressure effects on T_C were also observed for other iron-based SCs [3,11], suggesting an important role of the pressure which provides a controlled modification of superconducting properties without introducing the disorder effects by chemical substitution or doping.

There is growing anticipation that superconductivity is driven by spin fluctuations due to proximity to magnetic instability in these compounds [2,12]. The itinerant spin-density-wave (SDW) transitions were established in parent compounds of the Fe-based SCs, which are resulted in relatively small ordered magnetic moments, and in essentially non-Curie-Weiss behavior of magnetic susceptibility χ with temperature above T_{SDW} [4,5]. On the other hand, the undoped FeTe compound is not superconducting but magnetically ordered [6], and it was suggested that in FeTe the local magnetic moments interact via short-range superexchange [4,5].

There is still a controversy regarding an interplay between electronic structure, magnetism and superconductivity in the iron-based SC compounds. Therefore, further studies of magnetic and superconducting properties and their evolution with pressure can help to elucidate a mechanism of the superconductivity in the Fe-based SCs. In particular, the studies of pressure effect on magnetic susceptibility of the iron-based SC systems can shed more light on the nature of their magnetism. We expect that corresponding pressure (or volume) derivatives of χ are especially sensitive to the mechanism of magnetic interactions. The main objective of this study is to investigate atomic volume and pressure effects on magnetic properties of the LaFeAsO and $\text{FeSe}_{1-x}\text{Te}_x$ systems, which demonstrate a substantial pressure effect on T_C . The corresponding *ab initio* calculations of the electronic structure and magnetic susceptibility are supplemented by analysis of available experimental data.

The experimental data on magnetic susceptibility behavior of iron-based SCs in the normal state are still incomplete and contradictory [4–6]. In particular, the magnetic behaviors of $\text{FeSe}_{1-x}\text{Te}_x$ systems are substantially complicated by the presence of magnetic impurities and secondary phases. Therefore, it is very important to obtain the intrinsic susceptibility of the Fe-based SCs, in order to verify theoretical models, which can describe behavior of χ at ambient conditions and under pressure, and to elucidate effects of spin fluctuations.

In this work the polycrystalline $\text{LaFeAsO}_{0.85}\text{F}_{0.1}$ and $\text{FeSe}_{1-x}\text{Te}_x$ ($x \simeq 0$ and 1) samples were obtained by conventional solid-state synthesis. The single crystals $\text{FeSe}_{1-x}\text{Te}_x$ with $x \simeq 0.5$ and 1 were grown by slow cooling with the self-flux method, and two series of samples have been prepared. The phase content of the samples was checked by the X-ray diffraction method. Hereafter, we will refer to

the polycrystalline and single-crystalline samples of $\text{FeSe}_{1-x}\text{Te}_x$ as P and S , respectively, followed by the series number. The dc magnetization studies were carried out in the magnetic field up to 50 kOe and the temperature range 4.2–300 K using a superconducting quantum interference device (SQUID) magnetometer. For single crystals the magnetic field was applied along the tetragonal c -axis.

As seen in Fig. 1, the studied sample $\text{LaFeAsO}_{0.85}\text{F}_{0.1}$ shows the superconducting transition at temperature $T_C \approx 26$ K. For the normal state, the $\chi(T)$ dependence, measured in $H \geq 1$ T, appears to be relatively flat and roughly described by the mean value of $\chi_{av} \sim 5 \cdot 10^{-4}$ emu/mol. The peculiar feature of the low-field magnetic susceptibility of $\text{LaFeAsO}_{0.85}\text{F}_{0.1}$ is a clear cusp at $T \approx 135$ K with a sharp rise of χ with cooling from $T_M \approx 135$ K to $T_C \approx 26$ K.

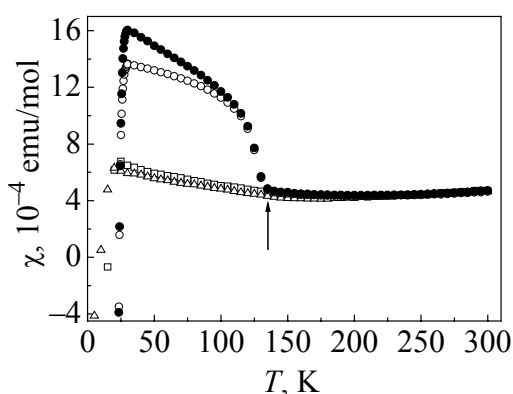


Fig. 1. Temperature dependences of dc magnetic susceptibility of $\text{LaFeAsO}_{0.85}\text{F}_{0.1}$ in different magnetic fields H , T: \square – 1.0, \triangle – 2.0, \circ – 0.02 [ZFC], \bullet – 0.02 [FC]; $T_M \approx 135$ K

Our magnetization $M(H)$ measurements on $\text{FeSe}_{1-x}\text{Te}_x$ have revealed a relatively large content of ferromagnetic (FM) impurities in the studied samples. In high magnetic fields the $M(H)$ dependences show a linear behavior with a slope determined by the intrinsic magnetic susceptibility of the samples. By their extrapolation to the zero field we have obtained the saturation moment values of FM impurities in our samples, which fall in the range from 25 to 300 emu/mol, being weakly dependent on temperature (see Table).

Table

Superconducting transition temperature T_C (in K), FM impurity saturation magnetic moment M_S (emu/mol) and host (intrinsic) magnetic susceptibility χ (10^{-3} emu/mol) at room and zero temperatures for $\text{FeTe}_{1-x}\text{Se}_x$ compounds

Compound	T_C	M_S	χ	
			290 K	0 K
$\text{FeSe}_{0.963}$ (P)	~ 7	214	0.5 ± 0.1	0.75 ± 0.1
$\text{FeSe}_{0.5}\text{Te}_{0.5}$ (S1)	13.5	280	1.3 ± 0.2	1.45 ± 0.2
$\text{FeSe}_{0.5}\text{Te}_{0.5}$ (S2)	14.2	9	0.85 ± 0.1	0.4 ± 0.1
$\text{FeTe}_{0.95}$ (P)	–	24	2.7 ± 0.2	2.65 ± 0.2
FeTe (S1)	–	103	2.9 ± 0.2	3.6 ± 0.2
FeTe (S2)	–	~ 0	5.7 ± 0.2	5.45 ± 0.2

Despite the pronounced FM impurities effects, the obtained magnetization data made it possible to estimate with sufficient accuracy the host (intrinsic) magnetic susceptibilities χ_{host} for $\text{FeSe}_{1-x}\text{Te}_x$ samples from the slope of linear part of corresponding $M(H)$ dependence in high fields. The resulted values of χ_{host} at some fixed temperatures are shown by full circles in Fig. 2. In the figure we also present the detailed $\chi_{\text{host}}(T)$ data, which were obtained according to the equation

$$\chi(T) \equiv \chi_{\text{host}}(T) = (M(T) - M_S) / H, \quad (1)$$

from temperature dependence of the magnetization $M(T)$ of $\text{FeSe}_{1-x}\text{Te}_x$ measured in magnetic field of 30 kOe. Here the saturation moment value M_S of FM impurity is assumed to be constant and equal to its temperature-averaged value for a given sample. The experimentally obtained basic superconducting and magnetic characteristics of the $\text{FeSe}_{1-x}\text{Te}_x$ samples are summarized in Table.

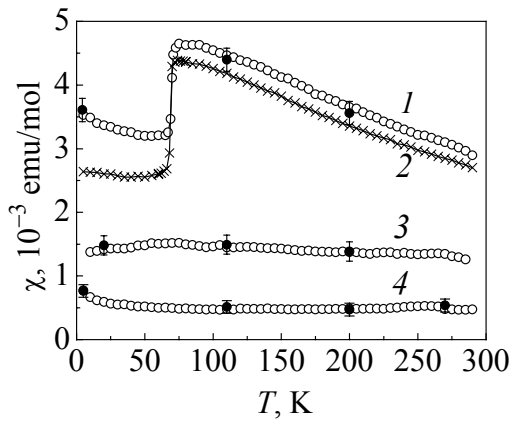


Fig. 2. Temperature dependence of the host magnetic susceptibility for some $\text{FeSe}_{1-x}\text{Te}_x$ compounds: 1 – FeTe (S1), 2 – $\text{FeTe}_{0.95}$ (P), 3 – $\text{FeTe}_{0.5}\text{Se}_{0.5}$ (S1), 4 – $\text{FeSe}_{0.963}$ (P). Full circles correspond to values derived from the high-field magnetization data

To gain a further insight into magnetic properties of the iron-based SC systems in the normal state, the *ab initio* calculations of the electronic structure and paramagnetic susceptibility are carried out for LaFeAsO , FeSe and FeTe parent compounds within the density functional theory (DFT). The calculations were performed for varying atomic volume at the corresponding experimental lattice parameter ratios c/a .

Under ambient conditions LaFeAsO and $\text{FeSe}_{1-x}\text{Te}_x$ compounds possess the tetragonal crystal structure (space group $P4/nmm$). The crystal lattice is composed of alternating slabs, which are stacked along the c -axis. Each iron layer is sandwiched between two chalcogen/pnictogen layers, which form edge-shared tetrahedrons around the iron sites. The positions of As (or Se/Te) sheets are fixed by the internal parameter Z , which represents the height of these atoms above the iron square plane. This parameter also determines the chalcogen-Fe bond angles. Crystal structure parameters of LaFeAsO and $\text{FeSe}_{1-x}\text{Te}_x$ compounds were established in a number of works by means of X -ray and neutron diffraction studies [1,5–7].

The previous *ab initio* calculations of the electronic structure of the «1111»- and «11»-type iron-based SCs were predominantly related to studies of the AFM

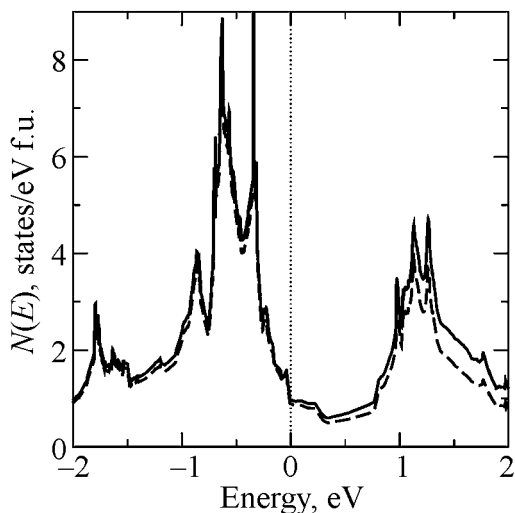


Fig. 3. Total density of states of the paramagnetic FeSe around E_F (solid line) and the partial contribution of the iron d -states (dashed line). The Fermi level position (at 0 eV) is marked by a vertical line

and SDW ordering (e.g. Refs. [12–14]). In this work the electronic structure calculations are carried out for LaFeAsO, FeSe and FeTe compounds with the aim to study a paramagnetic response in an external magnetic field, and to elucidate a nature of pressure effect on paramagnetism and magnetic instability. The *ab initio* calculations are carried out by employing a full-potential all-electron relativistic linear muffin-tin orbital method (FP-LMTO, code RSPt [15,16]). No shape approximations were imposed on the charge density or potential, what is especially important for the layered crystal structures. The exchange-correlation potential was treated within the local spin density approximation (LSDA, [17]) of the DFT.

The calculated basic features of electronic structure of LaFeAsO, FeSe and FeTe are in a qualitative agreement with results of earlier calculations [12–14]. In particular, the detailed density of states (DOS) $N(E)$ of FeSe is presented in Fig. 3. In the vicinity of the Fermi level E_F the d -states of Fe provide the dominant contribution to DOS in the range -2 eV and 2 eV around $E_F = 0$. The p states of chalcogen/pnictogen atoms are predominantly extended in the interstitial region, and their partial contributions to DOS in vicinity of E_F are substantially smaller for FeSe, FeTe and LaFeAsO. As seen in Fig. 3, in FeSe the Fermi level lies at the steep slope of $N(E)$ at the beginning of a pseudogap of about $\simeq 0.7$ eV. The evaluated for LaFeAsO, FeSe and FeTe volume derivatives $d \ln N(E_F) / d \ln V$ are found to be positive and equal to 0.94, 1.25 and 1.42, respectively, suggesting the decrease of $N(E_F)$ with uniform reduction of the unit cell volume.

The FP-LMTO-LSDA calculations of the field-induced spin and orbital (Van Vleck) magnetic moments were carried out for LaFeAsO, FeSe and FeTe self-consistently within the procedure described in Ref. [16] by means of the Zeeman operator

$$H_Z = \mu_B \mathbf{H} (2\hat{\mathbf{s}} + \hat{\mathbf{l}}) \quad (2)$$

which was incorporated in the original FP-LMTO Hamiltonian. Here \mathbf{H} is the external magnetic field, $\hat{\mathbf{s}}$ and $\hat{\mathbf{l}}$ – the spin and orbital angular momentum operators, respectively. For the tetragonal LaFeAsO, FeSe, and FeTe the paramagnetic contributions χ_{spin} and χ_{orb} were derived from the field-induced spin and orbital magnetic moments calculated in an external field of 10 T, which was applied parallel and perpendicular to the c -axis. The evaluated magnetic anisotropy, which is determined by the orbital con-

tribution, appeared to be negligible. The orbital Van Vleck contribution itself is substantially smaller (about 10%) than the strongly enhanced spin susceptibility χ_{spin} .

The calculated behavior of the field-induced magnetization in LaFeAsO is presented in Fig. 4. Due to the close proximity of the induced spin-polarized state to the spontaneous magnetic ordering for the experimental lattice parameters, the calculated total magnetic moment rises to $\approx 0.2\mu_B$, which in fact is close to the experimentally observed magnetic moment of $0.36\mu_B$ at Fe site in the AFM state [5]. As seen in Fig. 4, the spontaneous spin polarization occurs in the field-induced calculations at cell volumes above the theoretical value V_{LSDA} , whereas for $V \leq a_{\text{LSDA}}$ (approximately 6% lower than the experimental value), a paramagnetic response was obtained. For the theoretical equilibrium volume the contributions χ_{spin} and χ_{orb} are found to be equal to $0.545 \cdot 10^{-3}$ emu/mol and $0.046 \cdot 10^{-3}$ emu/mol, respectively.

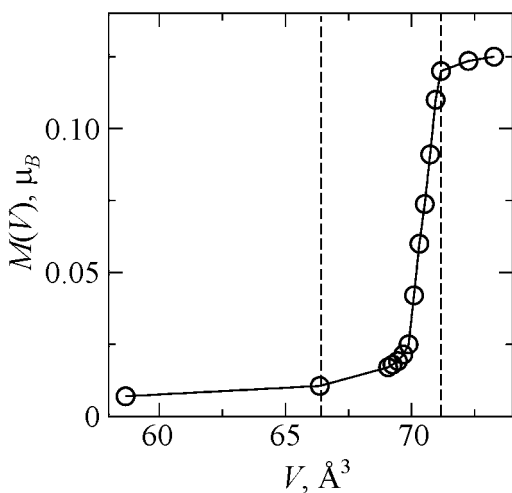


Fig. 4. Magnetic moment induced in the undoped LaFeAsO in the field of $H = 10$ T as a function of the cell volume with c/a and Z parameters fixed to their experimental ambient pressure values. Dashed vertical lines denote the calculated LSDA equilibrium volume and the experimental volume of LaFeAsO (from left to right)

For FeSe and FeTe the magnetic response to the external field appeared to be very sensitive to the height Z of chalcogen species from the Fe plane. The corresponding calculated dependences of magnetic susceptibility for FeSe and FeTe are given in Figs. 5 and 6, respectively. We can estimate the contributions to χ of FeSe as $\chi_{\text{spin}} = 0.55 \cdot 10^{-3}$ emu/mol and $\chi_{\text{orb}} = 0.11 \cdot 10^{-3}$ emu/mol for the experimental values of lattice parameters and Z ($Z = 0.26$ [7]). Therefore the calculated field-induced magnetic moments are in agreement with the experimental susceptibility of FeSe in the normal state (Table).

The itinerant nature of the hybridized $3d$ -states of Fe is an essential condition for the field-induced calculations of paramagnetic susceptibility. There is a strong experimental support of this itinerant picture for FeSe, which is expected to be in a non-magnetic spin-degenerate state [5]. For FeTe, however, a validity of the field-induced calculations of χ is questionable due to the expected more localized nature of the $3d$ -states. Therefore, the calculations for FeTe are performed only for volumes smaller than the experimental volume, and results of these calculations have to be thoroughly verified by other methods, and compared with experimental data.

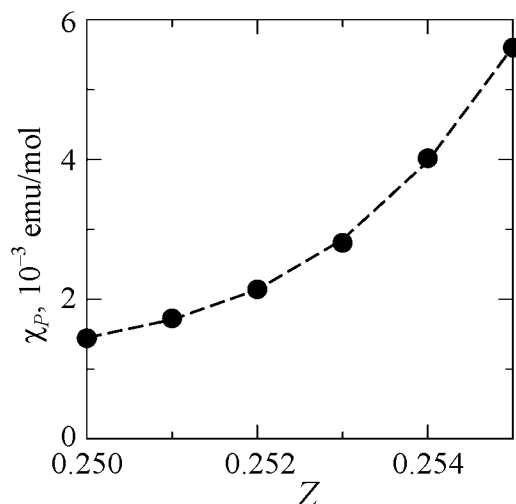
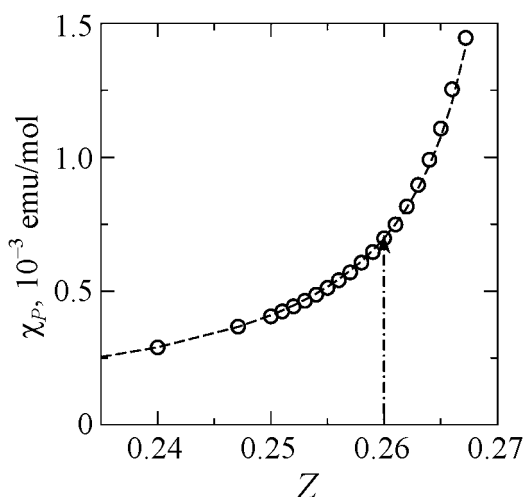


Fig. 5. Calculated paramagnetic susceptibility of FeSe as a function of the internal lattice parameter Z . The unit cell volume and c/a ratio are fixed to their experimental ambient pressure values (78.4 \AA^3 and 1.464, [7]). The dashed line is a guide for the eye. The dashed-dotted line corresponds to the experimental value of Z

Fig. 6. Calculated paramagnetic susceptibility of FeTe as a function of the internal lattice parameter Z for LSDA optimized (87 \AA^3) unit cell volume. The c/a ratio is fixed to the experimental ambient pressure value (1.647 [7]). The dashed line is a guide for the eye

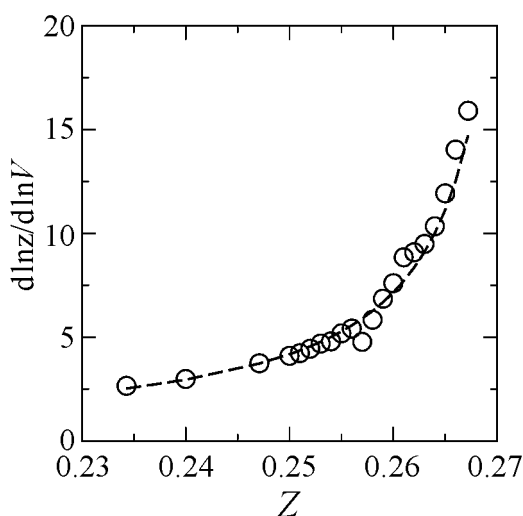


Fig. 7. Calculated volume dependence of the paramagnetic susceptibility $d \ln \chi / d \ln V$ of FeSe as a function of the internal lattice parameter Z . The c/a ratio is fixed to the experimental ambient pressure value (1.464 [7]). The dashed line is a guide for the eye

The calculated for FeSe magnetovolume effect $d \ln \chi / d \ln V$ is presented in Fig. 7. It sharply increases with Z and reaches the values consistent with magnetovolume effects in transition metals and compounds having substantially exchange-enhanced paramagnetic susceptibility (e.g. Pd, Sc, TiCo, Ni₃Al, YNi₅ [16,18,19]). This means that FeSe compound is on the verge of magnetic instability and close to a quantum critical point, which can result in strong spin fluctuations.

Within the experimental errors, the obtained data in Table indicate a gradual increase in magnetic susceptibility for FeSe_{1-x}Te_x system with increasing of tellurium content. For FeTe compound the paramagnetic state is unstable, and conver-

gence of the self-consistent field-induced LSDA calculations was actually obtained only for reduced lattice parameters. This is especially relevant to parameter Z , which had to be also reduced for about 10%. Therefore one should consider the calculated paramagnetic susceptibility of FeTe in Fig. 6 as a rough estimation which presumably allows to establish a trend for the effect of parameter Z . To further address the question whether a qualitative agreement between the calculated χ and experimental data for FeTe in Table I might be fortuitous, the detailed study of pressure effect on χ is highly desirable.

In conclusion, the superconducting transitions are detected at 8 and 13.6–14.2 K in FeSe_{0.963} and FeSe_{0.5}Te_{0.5} samples, respectively. Magnetic susceptibility of FeSe_{1-x}Te_x ($x \simeq 0, 0.5$ and 1.0) compounds was investigated in the temperature range 4.2–300 K, and the intrinsic χ in the series of iron chalcogenides FeSe_{0.963}, FeSe_{0.5}Te_{0.5} and FeTe is estimated to increase gradually ten times as much with Te content.

Ab initio calculations of the electronic structure and paramagnetic contributions to susceptibility of FeSe compound have revealed that this system is in close proximity to a quantum critical point, and this nearness can result in strong spin fluctuations. The paramagnetic susceptibility calculated in external magnetic field appears to be close to the experimental value for FeSe. These results point out that itinerant magnetism theory is relevant to describe magnetic properties of FeSe system. For both FeSe and FeTe, the LSDA calculated paramagnetic susceptibilities reveal a large magnetovolume effect and a drastic sensitivity to the structural parameter Z . Therefore, the experimental study of pressure effect on χ would be very useful to further address the question about a nature of paramagnetic state in FeSe_{1-x}Te_x.

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ВПЛИВ ТИСКУ НА ЕЛЕКТРОННУ БУДОВУ ТА МАГНІТНІ ВЛАСТИВОСТІ НАДПРОВІДНИКІВ НА ОСНОВІ ЗАЛІЗА З ВИСОКИМИ ЗНАЧЕННЯМИ T_C

Досліджено вплив тиску на електронну структуру та магнітні властивості надпровідників на основі заліза $\text{FeSe}_{1-x}\text{Te}_x$ ($x \approx 0, 0.5$ та 1.0) й LaFeAsO . Перехід в надпровідний стан в сполуках $\text{FeSe}_{0.963}$, $\text{FeSe}_{0.5}\text{Te}_{0.5}$ й $\text{LaFeAsO}_{0.85}\text{F}_{0.1}$ спостерігався відповідно при $T_C \approx 8, 13.6\text{--}14.2$ та 26 К. Визначено, що притаманна сполукам магнітна сприйнятливості χ в ряду $\text{FeSe}_{0.963}$, $\text{FeSe}_{0.5}\text{Te}_{0.5}$ й FeTe поступово збільшується приблизно на порядок величини зі зростанням концентрації телуру. Для сполуки $\text{LaFeAsO}_{0.85}\text{F}_{0.1}$ на виміряній в слабкому полі залежності $\chi(T)$ виявлена особливість у вигляді зламу поблизу температури $T_M \approx 135$ К. Для досліджуваних сполук здійснено *ab initio* розрахунки електронної структури й парамагнітної сприйнятливості в залежності від атомного об'єму і структурного параметру Z , що визначає висоту атомів халькогену відносно площини атомів заліза. Розрахунки індукованих полем магнітних моментів та їх об'ємних похідних вказують на близькість цих сполук до квантової критичної точки. Для сполук FeSe й FeTe розраховані парамагнітні сприйнятливості виявляють значний магнітооб'ємний ефект та екстремальну чутливість до параметру Z .

Ключові слова: FeAs-надпровідники, FeSe(Te)-сполуки, ефект тиску, намагніченість, електронна структура

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ВЛИЯНИЕ ДАВЛЕНИЯ НА ЭЛЕКТРОННУЮ СТРУКТУРУ И МАГНИТНЫЕ СВОЙСТВА ВЫСОКОТЕМПЕРАТУРНЫХ СВЕРХПРОВОДНИКОВ НА ОСНОВЕ ЖЕЛЕЗА

Изучены эффекты давления на электронную структуру и магнитные свойства сверхпроводников на основе железа $\text{FeSe}_{1-x}\text{Te}_x$ ($x \approx 0, 0.5$ и 1.0) и LaFeAsO . Переход в сверхпроводящее состояние в соединениях $\text{FeSe}_{0.963}$, $\text{FeSe}_{0.5}\text{Te}_{0.5}$ и $\text{LaFeAsO}_{0.85}\text{F}_{0.1}$ наблюдался соответственно при $T_C \approx 8, 13.6\text{--}14.2$ и 26 К. Установлено, что присущая соединениям магнитная восприимчивость χ в ряду $\text{FeSe}_{0.963}$, $\text{FeSe}_{0.5}\text{Te}_{0.5}$ и FeTe монотонно возрастает примерно на порядок величины с повышением концентрации теллура. Для соединения $\text{LaFeAsO}_{0.85}\text{F}_{0.1}$ в измеренной в слабом поле зависимости $\chi(T)$ была обнаружена особенность в виде излома при $T_M \approx 135$ К. Для исследуемых соединений выполнены *ab initio* расчеты электронной структуры и парамагнитной восприимчивости в зависимости от атомного объема и структурного параметра Z , который определяет относительную высоту атомов халькогена над плоскостью железа. Расчеты индуцированных полем магнитных моментов и их объемных производных указывают на близость этих соединений к квантовой критической точке. Для соединений FeSe и FeTe рассчитанные парамагнитные восприимчивости свидетельствуют о значительном магнитообъемном эффекте и сильной чувствительности к структурному параметру Z .

Ключевые слова: FeAs сверхпроводники, FeSe(Te)-соединения, эффект давления, намагниченность, электронная структура