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PRESSURE EFFECTS ON ELECTRONIC STRUCTURE AND MAGNETIC PROPERTIES OF THE FeSe(Te) SUPERCONDUCTORS

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The magnetic susceptibility χ of the FeSe and FeTe compounds, which form the simplest FeSe(Te) system of the novel iron-based superconductors, is studied in the normal state under hydrostatic pressure. A substantial positive pressure effect on χ is detected at low temperatures for both compounds. At room temperature, this effect is found to be also strong, but it is negative for FeSe and positive for FeTe. Ab initio calculations of the pressure dependent electronic structure and magnetic susceptibility indicate that FeSe and FeTe are close to magnetic instability with dominating enhanced spin paramagnetism. The calculated paramagnetic susceptibility exhibits a strong dependence on the unit cell volume and the height Z of chalcogen species from the Fe plane. The observed large positive pressure effects on χ in FeTe and FeSe at low temperatures are related to considerable sensitivity of the paramagnetism to the internal parameter Z . It is shown that available experimental data on the strong and nonmonotonic pressure dependence of the superconducting transition temperature in FeSe correlate qualitatively with the calculated behavior of the density of electronic states at the Fermi level.

Keywords: iron-based superconductors, FeSe, FeTe, magnetic susceptibility, pressure effect, electronic structure

1. Introduction

The novel superconducting FeSe_{1-x}Te_x compounds have attracted extensive attention due to the simplest crystal structure among the new families of iron-

based layered compounds exhibiting high temperature superconductivity (see Refs. [1,2] and references therein). This structural simplicity favors experimental and theoretical studies of chemical substitution and high pressure effects, which are aimed at better understanding of a mechanism of the superconductivity, and also at modifying properties of the novel superconducting materials.

For the $\text{FeSe}_{1-x}\text{Te}_x$ compounds, a nonmonotonic behavior of the superconducting transition temperature with x was found, rising from $T_C \sim 8$ K at $x = 0$ to a maximum value of ~ 15 K at $x \approx 0.5$. Additionally, a large enhancement of T_C up to 35–37 K was observed in FeSe under high pressures $P \approx 90$ kbar, indicating that FeSe is indeed a high temperature superconductor [3,4]. Similar pressure effects on T_C have been also reported for $\text{FeSe}_{0.5}\text{Te}_{0.5}$ [1].

The parent compound FeTe is not a superconducting one, but it exhibits peculiar magnetic properties. A drastic drop in the temperature dependence of its magnetic susceptibility $\chi(T)$ with decreasing temperature was observed at $T \approx 70$ K, which is related to the first-order structural phase transition accompanied by the onset of antiferromagnetic (AFM) order [1,2]. Though the attempts to obtain a superconducting phase in FeTe under high pressure appeared to be unsuccessful, the superconductivity at 13 K was detected by applying tensile stress conditions in thin films of FeTe, which involved in-plane extension and out-of-plane contraction of the lattice [5].

The tetragonal phase $P4/nmm$ of FeSe undergoes a weak distortion upon cooling to the lower symmetry orthorhombic $Cmma$ phase [3,6]. This transition occurs within a broad temperature range, about 70–100 K, depending on stoichiometry of the FeSe_{1-x} samples. Also, the tetragonal FeSe undergoes structural transitions under high pressures ($P \gtrsim 100$ kbar) to the hexagonal non-superconducting $P6_3mmm$ NiAs-type phase, and then to its orthorhombic modification ($Pbnm$, MnP-type) [3,7,8].

Though a substantial increase of T_C was observed in FeSe under pressure [3,9–11], these studies did not detect any trace of magnetic ordering. However, recent NMR studies provided some indication of magnetic phase transition under pressure [12]. Recently, a static magnetic ordering has been observed above $P \sim 100$ kbar by means of zero-field muon spin rotation (ZF μ SR) and neutron diffraction [13]. These studies indicated that as soon as magnetic ordering emerges, the magnetic and the superconducting states coexist, and both the transition temperatures grow simultaneously with increasing pressure.

Also, it was found that upon applying a pressure, the increase of T_C in FeSe_{1-x} appeared to be nonmonotonic and exhibits a local maximum at $P \approx 8$ kbar, which is followed by a local minimum at $P \approx 12$ kbar [9,10,13]. Thus, there is still a controversy regarding an interplay between electronic structure, magnetism and superconductivity in FeSe(Te) compounds. In order to elucidate the role of ex-

pected spin fluctuations in superconductivity, it is very important to investigate the nature of magnetism in FeSe and FeTe and its evolution with temperature and pressure.

Here we report results of detailed experimental studies of the effect of hydrostatic pressure on magnetic susceptibility of FeSe and FeTe compounds in the normal state. The experimental investigations are supplemented by *ab initio* calculations of the electronic structure and magnetic susceptibility of FeSe and FeTe within the density functional theory (DFT).

2. Experimental details and results

The single crystals of FeSe_{1-x} superconductor were grown in evacuated quartz ampoules using the KCl/AlCl₃ flux technique at stationary gradient of temperature. The energy dispersive X-ray spectroscopy revealed the FeSe_{0.95} composition, labelled in the following as FeSe for simplicity. The FeTe single crystal was grown by a slow-cooling self-flux method [14] and polycrystalline FeTe_{0.95} was prepared by a conventional solid-state synthesis. The tetragonal *P4/nmm* structure was checked by X-ray diffraction technique.

Magnetic properties of the samples were tested at $T = 4.2\text{--}300$ K by using SQUID magnetometer. For FeSe, the superconducting transition is detected in the range of 6–8 K. The magnetization dependencies of the samples in magnetic field up to 5 T appeared to be close to linear, indicating that concentrations of ferromagnetic impurities are negligibly small.

The temperature dependence of magnetic susceptibility $\chi(T)$ of the FeSe single crystal, measured in magnetic field around $H \approx 1$ T, is shown in Fig. 1. As is seen, a substantial growth of susceptibility with temperature was revealed in the normal state of FeSe, as well as large magnetic anisotropy. The figure also shows the $\chi(T)$ dependence for the FeSe sample, which includes about 50 small arbitrarily oriented single crystals. This sample, further called as «polycrystalline» FeSe, was used for study of the pressure effect on the magnetic susceptibility. In Fig. 2 the measured temperature dependencies $\chi(T)$ are shown for the FeTe single crystal ($H||c$) and for the polycrystalline FeTe_{0.95}. The data exhibit a distinct peculiarity at $T \approx 70$ K, which is presumably related to simultaneous structural and magnetic transition [2].

The study of magnetic susceptibility under helium gas pressure P up to 2 kbar was performed at fixed temperatures of 78 and 300 K by using a pendulum-type magnetometer placed directly in the nonmagnetic pressure cell [16]. High level of hydrostaticity of pressure is essential to obtain sufficiently precise pressure dependencies of χ , because FeSe and FeTe have inhomogeneous compressibilities associated with the layered structure. The measurements were carried out in the field $H = 1.7$ T and their relative errors did not exceed 0.5% for FeSe sample and 0.2% for FeTe one. The experimental pressure dependencies $\chi(P)$ at different temperatures are shown in

Figs. 3 and 4, which demonstrate a linear character. The obtained pressure effects on magnetic susceptibility $d\ln\chi/dP$ for the FeSe and FeTe compounds are compiled in Table 1.

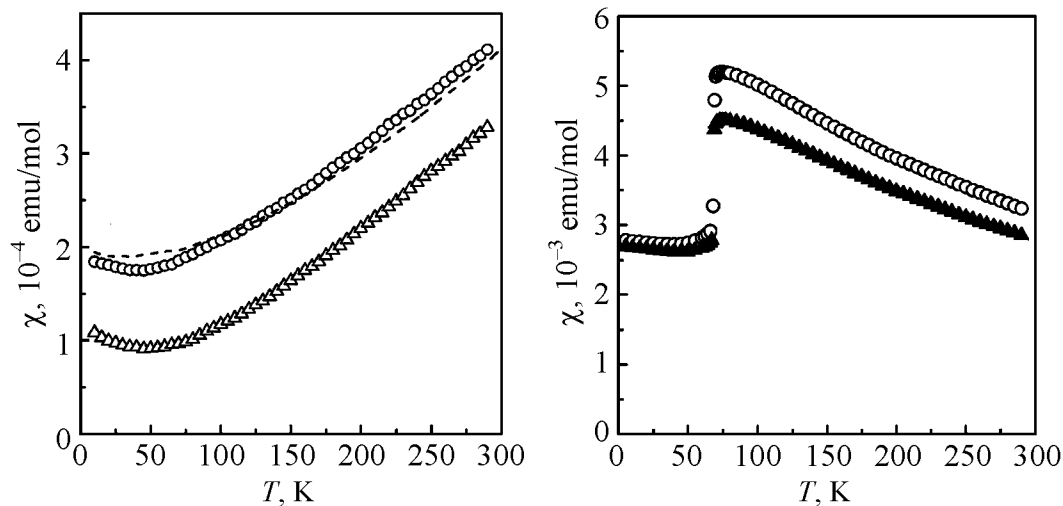


Fig. 1. Temperature dependencies of magnetic susceptibility in the normal state for the single-crystalline sample FeSe and the «polycrystalline» sample FeSe (dashed line). Data for the single crystal corresponding to magnetic field directions $H \perp c$ axis and $H \parallel c$ are denoted by \circ and Δ symbols, respectively

Fig. 2. Temperature dependence of the magnetic susceptibility for the FeTe single crystal (\circ) and the FeTe_{0.95} polycrystalline sample (\blacktriangle)

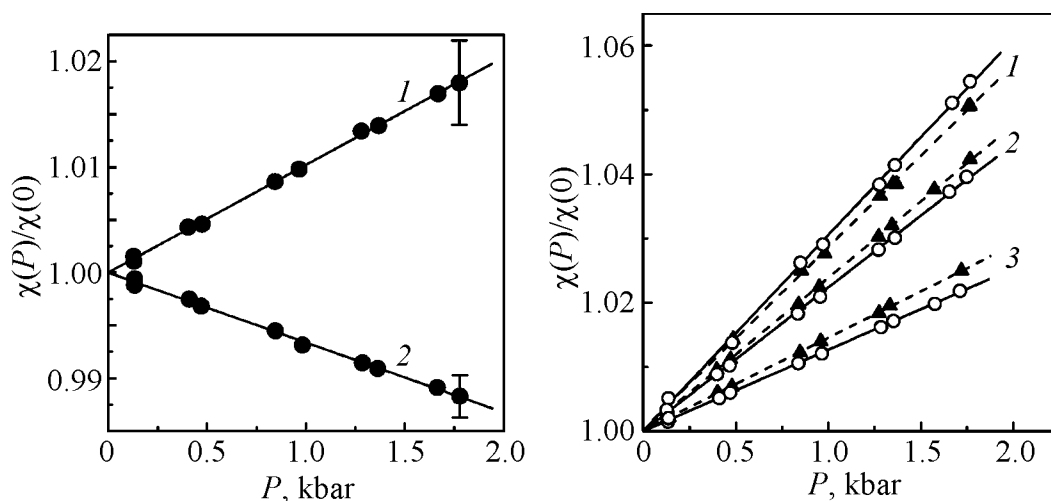


Fig. 3. Pressure dependencies of the magnetic susceptibility, normalized to its value at $P = 0$, for the «polycrystalline» FeSe compound at temperatures 78 (1) and 300 K (2). The solid lines are guides for the eye

Fig. 4. Pressure dependencies of the magnetic susceptibility, normalized to its value at $P = 0$, for the single-crystalline FeTe (solid line) and the polycrystalline FeTe_{0.95} (dashed line) compounds at temperatures, K: 1 – 55, 2 – 78, 3 – 300

Table 1

Pressure effect on magnetic susceptibility $d\ln\chi/dP$ for the FeSe and FeTe compounds

Method	T, K	$d\ln\chi/dP$, Mbar ⁻¹	
		FeSe	FeTe
Experiment	78	10 ± 3	23 ± 1.5
	300	-6.5 ± 1	13 ± 1
Theory	≈ 10	≈ 12	~ 20
Theory*	≈ 10	≈ 8	–

*Present calculations with structural parameters from Ref. [15].

3. Computational details and results

Ab initio calculations of the electronic structure and paramagnetic susceptibility were aimed at the pressure effect on magnetic properties of FeSe and FeTe compounds in the normal state. At ambient conditions these compounds possess the tetragonal PbO-type crystal structure (space group $P4/nmm$), which is composed by alternating triple-layer slabs. Each iron layer is sandwiched between two nearest-neighbor layers of chalcogen atoms, which form edge-shared tetrahedron around the iron sites. The positions of layers are fixed by the structural parameter Z , which represents the relative height of chalcogen atoms above the iron plane. The structural parameters of FeSe and FeTe were determined by means of X-ray and neutron diffraction and given in Refs. [1–3,6,8,17,18].

The purpose of the present calculations was evaluation of the paramagnetic response in an external magnetic field and elucidation of the nature and features of magnetism in the FeSe and FeTe compounds. The electronic structure calculations were performed by employing a full-potential linear muffin-tin orbital method (FP-LMTO, code RSPt [19]). The exchange-correlation potential was treated within the local spin density approximation. The calculated basic features of electronic structures of FeSe and FeTe are in a qualitative agreement with the results of previous calculations (see Refs. [15,20]).

To evaluate the paramagnetic susceptibilities of FeSe and FeTe, FP-LMTO calculations of the field-induced spin and orbital (Van Vleck) magnetic moments were carried out within the approach described in Refs.[21,22]. The spin-orbit coupling was incorporated, and the effect of an external magnetic field \mathbf{H} was taken into account self-consistently by means of the Zeeman term:

$$H_Z = \mu_B \mathbf{H} (2\hat{\mathbf{s}} + \hat{\mathbf{l}}). \quad (1)$$

Here μ_B is the Bohr magneton, $\hat{\mathbf{s}}$ and $\hat{\mathbf{l}}$ are the spin and orbital angular momentum operators, respectively. The induced in the external field of 10 T spin and orbital magnetic moments provide the related contributions to the magnetic susceptibility, χ_{spin} and χ_{orb} .

It is found that magnetic response to the external field is very sensitive to the unit cell volume, as well as to the internal parameter Z . The calculated dependen-

cies of susceptibility of FeSe as functions of the volume and parameter Z are given in Figs. 5 and 6, respectively. The similar but more pronounced dependencies of susceptibility as those in Figs. 5 and 6 were also obtained for FeTe.

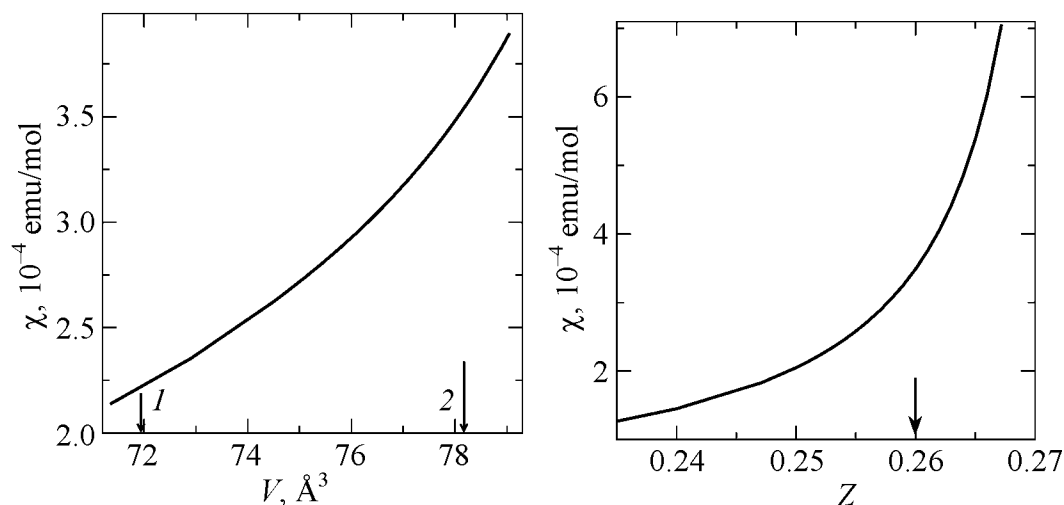


Fig. 5. Calculated paramagnetic susceptibility of FeSe as a function of unit cell volume. Z is taken to be 0.26. The arrows indicate the theoretical (1) and experimental (2) equilibrium volume values

Fig. 6. Calculated paramagnetic susceptibility of FeSe as a function of Z for the experimental unit cell volume

4. Discussion

Above T_C , a substantial growth of susceptibility with temperature was revealed in the normal state of FeSe up to 300 K (Fig. 1). This fact apparently indicates the itinerant nature of electronic states of Fe near E_F , however the scale of the effect is larger than might be expected. It is presumably related to a fine structure of DOS $N(E)$ at E_F , but one should expect that FeSe system is driven far from the ground state at room temperatures. As is seen in Fig. 2, in FeTe $\chi(T)$ exhibits an anomaly at $T \approx 70$, which is in agreement with the literature data [1,2] and apparently associated with the magnetic and structural transitions.

In order to analyse the experimental data on $\chi(P)$ in FeSe and FeTe, we used the calculated paramagnetic contributions to susceptibility, χ_{spin} and χ_{orb} . The orbital χ_{orb} term amounts to about 15% of the total paramagnetic susceptibility for FeSe and FeTe. The *ab initio* calculations of the paramagnetic susceptibility of the tetragonal FeSe and FeTe compounds revealed that these systems are in close proximity to the quantum critical point and magnetic instability (see Figs. 5 and 6), and this nearness can result in strong spin fluctuations.

In fact, for FeSe the calculated paramagnetic contribution $\chi_{\text{spin}} + \chi_{\text{orb}}$ has to be substantially compensated by a diamagnetic one in order to conform with the experimental data in Fig. 1. From comparison of the calculated paramagnetic susceptibilities in Figs. 5 and 6 with the experimental dependence of $\chi_{\text{exp}}(T)$ in Fig. 1, one

can estimate a diamagnetic contribution to magnetic susceptibility of FeSe to be about $-1.5 \cdot 10^{-4}$ emu/mol. This diamagnetism is comparable in absolute value with the paramagnetic contribution, and presumably comes from conduction electrons.

The observed large pressure effects on magnetic susceptibility of FeSe and FeTe are intriguing and require examination. Firstly, as can be seen in Fig. 3 and in Table 1, there is a striking sign difference for the pressure effects on χ in FeSe at low and room temperatures. Also, the absolute value of this effect is substantially larger than that observed in strongly enhanced itinerant paramagnets [22]. In FeTe the observed pressure effect on χ appeared to be even larger and *positive* at low and room temperatures (see Fig. 4 and Table 1).

In order to clarify mechanisms of the behavior of $\chi(P)$, we carried out field-induced *ab initio* calculations of paramagnetic susceptibility for FeSe in the range of 0–10 kbar, based upon the pressure dependent structural parameters obtained and listed in Ref. [15]. The corresponding calculated $Z(P)$ are in agreement with the experimental data [3,6,8,18], as is seen in Fig. 7. As a result, the calculated values of $d \ln \chi / dP$ for FeSe appeared to be in a qualitative agreement with the experimental low temperature data, see Table 1.

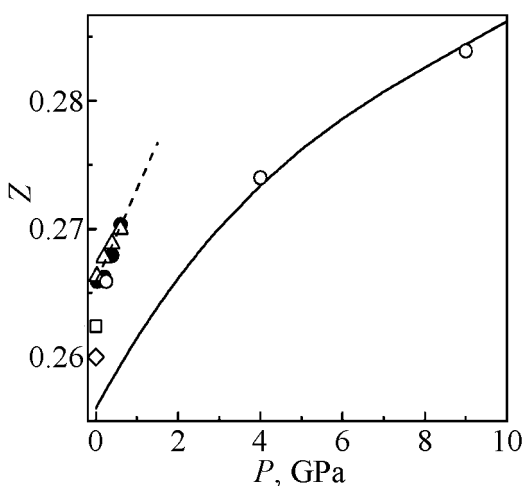


Fig. 7. Calculated pressure behavior of the internal chalcogen structural parameter Z for FeSe (taken from Ref. [15], solid line). Experimental data on parameter Z in FeSe for the tetragonal phase at $T = 190$ (Δ , [6]), 295 (\square , [17]) and 300 K (\diamond , [18]), and for the orthorhombic phase at $T = 16$ (\circ , [3]) and 50 K (\bullet , [6]). The dashed line is a guide for the eye

In order to elucidate the main mechanism of the experimentally observed strong increase in the magnetic susceptibility of FeSe and FeTe under pressure, we have also analyzed the pressure effect in terms of the corresponding change of the volume and Z parameters by using the relation:

$$\frac{d \ln \chi}{dP} = \frac{\partial \ln \chi}{\partial \ln V} \frac{d \ln V}{dP} + \frac{\partial \ln \chi}{\partial Z_X} \frac{dZ_X}{dP}. \quad (2)$$

The required values of the partial volume and Z derivatives of χ were estimated from the results of *ab initio* calculations (as those presented in Figs. 5 and 6 for FeSe), and were found to be $\partial \ln \chi / \partial \ln V \approx 8$ and $\partial \ln \chi / \partial Z \approx 65$ for FeSe, and $\partial \ln \chi / \partial \ln V \approx 40$ and $\partial \ln \chi / \partial Z \approx 350$ for FeTe. The value $d \ln V / dP = -3 \text{ Mbar}^{-1}$ is taken for the compressibility of FeSe and FeTe, which agrees closely with the experimental values reported in Refs. [4,6,7]. Also, the optimized value $dZ/dP = 0.55 \text{ Mbar}^{-1}$ [15] was

adopted for evaluation of Eq. (2). As is seen in Fig. 7, this value of dZ/dP at lower pressures is in agreement with the experimental data of Ref. [6]. The experiments of Ref. [3] were basically focused on the higher pressures (up to 120 kbar), and have not provided detailed data for the lower pressure region.

As far as all parameters entering Eq. (2) are estimated, the first term in (2) results in a large negative value of about -24 Mbar^{-1} , whereas the second term appears to be large and positive: $\partial \ln \chi / \partial Z \times dZ/dP \simeq 36 \text{ Mbar}^{-1}$. The both terms in Eq. (2) taken together yield the theoretical estimation $d \ln \chi / dP \simeq 12 \text{ Mbar}^{-1}$ for FeSe, which is qualitatively consistent with the low temperature experimental data and results of our direct *ab initio* calculations of $\chi(P)$ (see Table 1).

In the absence of reliable data on dZ/dP for FeTe, we can fit the experimental pressure effect $d \ln \chi / dP \sim 20 \text{ Mbar}^{-1}$ for FeTe in PM state within Eq. (2) by setting $dZ/dP = 0.40 \text{ Mbar}^{-1}$, which provides a large positive value of the second term in Eq. (2), $\partial \ln \chi / \partial Z \times dZ/dP \simeq 140 \text{ Mbar}^{-1}$. Actually, the above choice of the dZ/dP derivative is consistent with the available data on the pressure dependence of Z parameter for the related FeSe compound, as is seen in Fig. 7.

The above estimations allowed to shed light on the nature of the observed hydrostatic pressure effect on χ in FeTe and FeSe (at low temperatures) by separating effects of change in structural parameters V and Z . Based on results of the *ab initio* calculations, shown in Figs. 5 and 6, it is found that the pressure effect on χ for FeSe (and also for FeTe) can be represented as a sum of two large in size and competing contributions, related to the pressure dependence of the structural parameters V and Z . Therefore, the large *positive* values of the pressure effect $d \ln \chi / dP$ are determined by a change of Z under pressure, which plays a substantial role in Eq. (2), taking into account the calculated strong dependences of susceptibility on Z .

The nature of this large positive pressure effect on χ in FeSe is similar to that for FeTe compound. However, in the case of FeTe, such effect is twice more pronounced, and also takes place at room temperatures, whereas for FeSe $d \ln \chi / dP$ is found to be negative at 300 K (see Table 1). The grounds of this difference are unclear. At the present stage one can presume, that the negative sign of $d \ln \chi / dP$ derivative is probably related to the nature of the observed anomalous growth of $\chi(T)$ up to room temperatures (Fig. 1), which is not the case for FeTe.

Basically, the observed positive pressure effect on χ in FeSe at low temperatures correlates with the calculated behavior of the density of states at the Fermi level $N(E_F)$ at low pressures (Fig. 8). At higher pressures, one can see non-monotonic variation of $N(E_F)$ in Fig. 8 which clearly exhibits the consecutive maximum at 5 kbar and the minimum at 22 kbar. It should be noted, that the presently calculated behavior of $N(E_F)$ under pressure is qualitatively consistent with the reported experimental dependencies of $T_C(P)$ in FeSe (the corresponding maximum and minimum of $T_C(P)$ were observed at $\simeq 8$ kbar and $\simeq 13$ kbar, respectively [9,10,13]). This correlation of pressure dependencies of $N(E_F)$ and T_C might be considered as an indication of BCS-like pairing mechanism in FeSe.

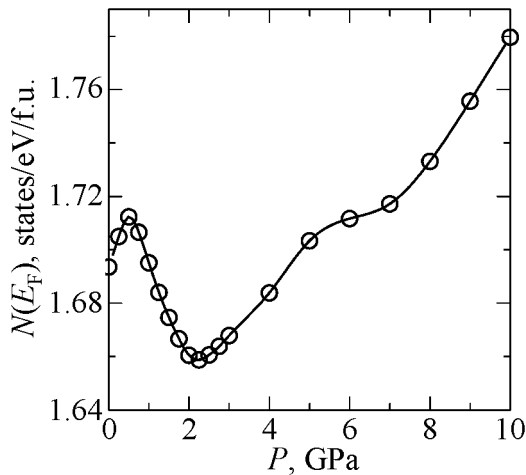


Fig. 8. Calculated pressure dependencies of the density of states at the Fermi level for FeSe (in states/eV/f.u.). The pressure dependent structural parameters, including lattice constants and atomic positions, were taken from the optimization of Ref. [15] (○) with the small upward shift $\Delta Z = +0.004$ to start from the experimental value of Z (see $Z(P)$ behavior in Fig. 7). The solid line is a guide for the eye

5. Conclusions

The intrinsic magnetic susceptibility of FeSe compound is found to rise substantially with temperature, which points to the itinerant nature of the electronic states of Fe. The origin of the observed about twofold increase of χ in FeSe up to 300 K is puzzling. The precision measurements of magnetic susceptibility were carried out under hydrostatic gaseous pressure and the strong positive pressure effect on χ is revealed for FeTe and for FeSe at low temperatures, whereas at room temperature for FeSe the pressure effect is found to be also strong, but *negative*.

Ab initio calculations of the paramagnetic susceptibility of FeSe and FeTe revealed that these systems are in close proximity to the quantum critical point, and this nearness can result in strong spin fluctuations. Paramagnetic susceptibility of FeSe and FeTe indicates a strong sensitivity to the unit cell volume V and the height Z of chalcogen species above the Fe plane. It is found that the observed large positive pressure effect on χ in FeSe at low temperatures and in FeTe is related to considerable sensitivity of the paramagnetic susceptibility to the internal parameter Z , determining the dominant positive term in Eq. (2). At higher temperatures, the anomalous growth of $\chi(T)$ in FeSe is apparently reduced by applied pressure, however the grounds of the negative sign of $d\ln\chi/dP$ derivative at 300 K are unclear.

The present calculations demonstrate that for the FeSe compound, the behavior of superconducting transition temperature with pressure correlates with the density of electronic states at the Fermi level. This fact indicates a possibility of realization of the BCS-like pairing mechanism in this system. In general, our results suggest that the itinerant magnetism approach within the DFT-LSDA methods is relevant to describe the paramagnetic normal state of FeSe and FeTe.

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ВПЛИВ ТИСКУ НА ЕЛЕКТРОННУ СТРУКТУРУ Й МАГНІТНІ ВЛАСТИВОСТІ НАДПРОВІДНИКІВ FeSe(Te)

Магнітну сприйнятливість χ сполук FeSe і FeTe, які утворюють найпростішу систему FeSe(Te) нових надпровідників на основі заліза, вивчено в нормальному стані під дією гідростатичного тиску. Значний позитивний ефект тиску на χ визначено при низьких температурах для обох сполук. При кімнатній температурі цей ефект виявляється також сильним, але негативним – для FeSe і позитивним – для FeTe. Розрахунки з перших принципів залежності електронної структури й магнітної сприйнятливості від тиску показали, що FeSe і FeTe близькі до магнітної нестійкості з переважанням обмінно-поширеного спінового парамагнетизму. Обчислена парамагнітна сприйнятливість проявляє сильну залежність від об'єму елементарної комірки й висоти Z шару халькогену над площиною заліза. Великі позитивні ефекти тиску на χ в FeTe і FeSe, які спостерігалися при низьких температурах, пов'язані зі значною чутливістю парамагнетизму до внутрішнього параметру Z . Показано, що наявні експериментальні дані про сильну й немонотонну залежність температурного надпровідного переходу від тиску в FeSe якісно корелюють із розрахованою поведінкою густини електронних станів на рівні Фермі.

Ключові слова: надпровідники на основі заліза, FeSe, FeTe, магнітна сприйнятливість, ефект тиску, електронна структура

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ВЛИЯНИЕ ДАВЛЕНИЯ НА ЭЛЕКТРОННУЮ СТРУКТУРУ И МАГНИТНЫЕ СВОЙСТВА СВЕРХПРОВОДНИКОВ FeSe(Te)

Магнитная восприимчивость χ соединений FeSe и FeTe, которые образуют простейшую систему FeSe(Te) новых сверхпроводников на основе железа, изучена в нормальном состоянии под действием гидростатического давления. Значительный положительный эффект влияния давления на χ обнаружен при низкой температуре для обоих соединений. При комнатной температуре этот эффект оказывается также сильным, но отрицательным – для FeSe и положительным – для FeTe. Расчеты из первых принципов зависимости электронной структуры и магнитной восприимчивости от давления показали, что FeSe и FeTe близки к магнитной неустойчивости с преобладанием обменно-усиленного спинового парамагнетизма. Вычисленная парамагнитная восприимчивость проявляет сильную зависимость от объема элементарной ячейки и высоты Z слоя халькогена над плоскостью железа. Наблюдаемые большие положительные эффекты давления на χ в FeTe и FeSe при низких температурах связаны со значительной чувствительностью парамагнетизма к внутреннему параметру Z . Показано, что имеющиеся экспериментальные данные о сильной и немонотонной зависимости температурного сверхпроводящего перехода от давления в FeSe качественно коррелируют с рассчитанным поведением плотности электронных состояний на уровне Ферми.

Ключевые слова: сверхпроводники на основе железа, FeSe, FeTe, магнитная восприимчивость, эффект давления, электронная структура