The electronic energy structures and magnetic properties of layered superconductors RNi$_2$B$_2$C, RFe$_4$Al$_8$, and FeSe are systematically studied, by using the density functional theory (DFT). The calculations allowed us to reveal a number of features of the electronic structure, which can cause the manifestation of peculiar structural, magnetic and superconducting properties of these systems. It is demonstrated that the Fermi energy $E_F$ is located close to the pronounced peaks of the electronic density of states (DOS). The main contribution to DOS at the Fermi level arises from 3$d$-electrons. The calculations of the pressure-dependent electronic structure and the magnetic susceptibility in the normal state indicate that the novel superconductors are very close to a magnetic instability with dominating spin paramagnetism. It is shown that experimental data on the pressure dependence of the superconducting transition temperature in FeSe correlate qualitatively with the calculated behavior of DOS at $E_F$ as a function of the pressure.

**Keywords:** Electronic structure, magnetic superconductors, RNi$_2$B$_2$C, RFe$_4$Al$_8$, FeSe.

1. Introduction

The discovery of the superconductivity in transition metal borocarbides with the general formula RNi$_2$B$_2$C ($R=\text{Y, Ho, Er, Tm or Lu}$) and its coexistence with magnetism stimulated a considerable scientific interest in these systems [1]. Later, the superconductivity was also found in magnetic compounds YFe$_4$Al$_8$, LuFe$_4$Al$_8$, and ScFe$_4$Al$_8$ at temperatures lower than 6 K [2]. In 2008, the new class of iron-based layered superconductors was discovered. One of the representatives of this class is FeSe compound distinguished by the simplest crystal structure among iron-based superconductors and by the extremely large effect of a pressure on the superconducting transition temperature [3–5].

The characteristic feature of these layered compounds of 3$d$-metals is the well-established coexistence of magnetism and superconductivity. The relative structural simplicity of RNi$_2$B$_2$C, RFe$_4$Al$_8$, and FeSe is favourable for studying the effects of chemical substitution, high pressure, and uniaxial deformations on their physical properties. Such studies can reveal a mechanism of superconductivity in these systems, which contain magnetic 3$d$-metals.

The clarification of microscopic mechanisms, which determine electric and magnetic properties of metallic systems, assumes detailed experimental and theoretical studies of the electronic structure of a conduction band. A number of electronic structure calculations were carried out for nickel borocarbides [6, 7] and superconducting FeSe [8, 9] in recent years. However, the data on the electronic energy structure of these systems are still incomplete and inconsistent.

In very recent studies of magnetic superconductors with the angular resolved photoemission spectroscopy method (ARPES) [10], the presence of Van Hove singularities was established in the electronic structures in a small vicinity of the Fermi energy $E_F$. Moreover,
the technological progress in growing single-crystal samples provided an opportunity to study the fine structure of the electronic energy bands and the Fermi surface of nickel borocarbides by means of the de Haas–van Alphen effect [11, 12] and ARPES [13] and FeSe compound (ARPES, [14]). Thus, the detailed ab initio calculations of the electronic structure are necessary for the analysis of the spectral characteristics of these systems.

Here, we have calculated the electronic band structures and a number of thermodynamic characteristics of $RNi_2B_2C$, $RFe_4Al_8$, and FeSe compounds within the density functional theory (DFT) methods. The dependences of these characteristics on the volume and structural parameters were addressed to shed light on the corresponding high-pressure effects.

### 2. Details and Results of Electronic Structure Calculations

The calculations of electronic structures were carried out by using the modified relativistic LMTO method with a full potential (FP-LMTO, RSPt implementation [15, 16]) and the linearized augmented plane waves method with a full potential (FP-LAPW, Elk implementation [17]). The exchange and correlation potentials were treated within the local density approximation (LDA [18]) and the generalized gradient approximation (GGA [19]) of DFT. For the employed full potential FP-LMTO and FP-LAPW methods, any restrictions were not imposed on the charge densities or potentials of the studied systems, which is especially important for anisotropic layered structures of the investigated magnetic superconductors.

Electronic structure calculations for compounds were carried out for the sets of crystal lattice parameters close to experimental ones. Variations of the parameters of crystal lattices allow one to imitate the influence of an external pressure. In such a way, the volume dependence of the total energy of the electronic subsystem, $E(V)$, was calculated for the studied compounds. The theoretical values of equilibrium lattice parameters and bulk moduli $B$ were determined from the calculated $E(V)$ dependences, by using the known Birch–Murnaghan equation of state (see Refs. [15, 16]).

To evaluate the paramagnetic susceptibility of compounds, the FP-LMTO calculations of field-induced spin and orbital (Van Vleck) magnetic moments were carried out with the approach described in Ref. [15] within the local spin density approximation (LSDA) of DFT. The relativistic effects, including spin-orbit coupling, were incorporated, and the effect of an external magnetic field $B$ was taken into account self-consistently by means of the Zeeman term,

$$\mathcal{H}_Z = \mu_B B \left( 2s + I \right).$$  \hspace{1cm} (1)

Here, $\mu_B$ is the Bohr magneton, and $s$ and $I$ are the spin and orbital angular momentum operators, respectively. The field-induced spin and orbital magnetic moments provide the related contributions to the magnetic susceptibility, $\chi_{\text{spin}}$ and $\chi_{\text{orb}}$.

### 2.1. $RNi_2B_2C$

The crystal structure of nickel borocarbides (like YNi$_2$B$_2$C, space group $I4/mmm$) is a body-centered tetragonal structure with alternating triple layers of B-Ni-B and Y-C planes. In this work, we carried out the DFT calculations of the band structures, densities of electronic states (DOS), and some thermodynamic characteristics of YNi$_2$B$_2$C, LaNi$_2$B$_2$C, and LuNi$_2$B$_2$C compounds. These compounds contain non-magnetic trivalent transition metals Y, La, and Lu, whose external electronic shells are similar to those of rare-earth elements $R$. For each compound, the calculations of the electronic structure were carried out for a number of lattice parameters, close to
experimental ones (listed in Refs. [1, 20]). At the
same time, the c/a ratio was fixed and corresponded
to the experimental value for each $RNi_2B_2C$ com-

The calculated densities of electronic states $N(E)$
of these nickel borocarbides are similar, but differ in
details and the positions of Fermi levels $E_F$ (see
Fig. 1). In Fig. 1, one can see the sharp peaks in
$N(E)$ of YNi$_2$B$_2$C and LuNi$_2$B$_2$C superconductors
in a close proximity of the Fermi level, whereas the
related peak in the non-superconducting LaNi$_2$B$_2$C
compound is situated much deeper below $E_F$.

The calculated band structure of YNi$_2$B$_2$C com-

The reliability of the present calculations of the
electronic structure of nickel borocarbides is con-

Fig. 2. Band structure of YNi$_2$B$_2$C along high symmetry lines
of the Brillouin zone. The Fermi level ($E = 0$) is marked by
the horizontal line

(see $E(k)$ dependences in Fig. 2). It should be noted
that, for a small shift of the Fermi level (less than
0.1 eV), which corresponds to the accuracy of the $ab$
initio calculations of the Fermi energy position, the

The difference of the estimated $\gamma_{\text{exp}}$ from Table 1, one can estimate the superconduct-

The calculated values of DOS at the Fermi level $N(E_F)$ for
the nickel borocarbides are presented in

By using the theoretical and experimental data
from Table 1, one can estimate the superconduct-

The value of $\mu^*$ is taken to be 0.13, as accepted for transitional
metals [23]. Thus, using the experimental values of
Debye temperatures $\Theta_D$ and estimated $\lambda$, we obtained
$T_c$ values, which are in a good agreement with experimental
data for YNi$_2$B$_2$C and LuNi$_2$B$_2$C (see Table 1). The difference of the estimated $T_c$ with
the experimental value for LaNi$_2$B$_2$C can be caused ei-

$\lambda = \lambda_{\text{el}} + \lambda_{\text{mf}}$,  

$$
\lambda_{\text{el}} = \frac{\Theta_D}{1.45 \exp \left[ - \frac{1.04(1 + \lambda)}{\lambda - \mu^*(1 + 0.62\lambda)} \right]},
$$

$$
\gamma_{\text{exp}} = (1 + \lambda)\gamma_{\text{theor}},
$$

$\lambda_{\text{el}}$ and $\lambda_{\text{mf}}$ correspond to the sharp peak of DOS in a vicinity of $E_F$
(see Table 1). The main contribution to $N(E_F)$ comes from the $d$-states of nickel
layers.

The reliability of the present calculations of the
electronic structure of nickel borocarbides is con-

$\Theta_D$ – Debye’s temperature, $\lambda$ – electron-
phonon interaction constant, and $\mu^*$ – Morel–
Anderson’s Coulomb pseudopotential. The value of
$\mu^*$ is taken to be 0.13, as accepted for transitional
metals [23]. Thus, using the experimental values of
Debye temperatures $\Theta_D$ and estimated $\lambda$, we obtained
$T_c$ values, which are in a good agreement with experimental
data for YNi$_2$B$_2$C and LuNi$_2$B$_2$C (see Table 1). The difference of the estimated $T_c$ with
the experimental value for LaNi$_2$B$_2$C can be caused ei-

The reliability of the present calculations of the
electronic structure of nickel borocarbides is con-

$\Theta_D$ – Debye’s temperature, $\lambda$ – electron-
phonon interaction constant, and $\mu^*$ – Morel–
Anderson’s Coulomb pseudopotential. The value of
$\mu^*$ is taken to be 0.13, as accepted for transitional
metals [23]. Thus, using the experimental values of
Debye temperatures $\Theta_D$ and estimated $\lambda$, we obtained
$T_c$ values, which are in a good agreement with experimental
data for YNi$_2$B$_2$C and LuNi$_2$B$_2$C (see Table 1). The difference of the estimated $T_c$ with
the experimental value for LaNi$_2$B$_2$C can be caused ei-

The reliability of the present calculations of the
electronic structure of nickel borocarbides is con-

$\Theta_D$ – Debye’s temperature, $\lambda$ – electron-
phonon interaction constant, and $\mu^*$ – Morel–
Anderson’s Coulomb pseudopotential. The value of
$\mu^*$ is taken to be 0.13, as accepted for transitional
metals [23]. Thus, using the experimental values of
Debye temperatures $\Theta_D$ and estimated $\lambda$, we obtained
$T_c$ values, which are in a good agreement with experimental
data for YNi$_2$B$_2$C and LuNi$_2$B$_2$C (see Table 1). The difference of the estimated $T_c$ with
the experimental value for LaNi$_2$B$_2$C can be caused ei-

which can explain a smaller contribution of $\lambda_{el-ph}$. Nevertheless, the results in Table 1 clearly testify in favor of the BCS-like electron-phonon mechanism of superconductivity in the nickel borocarbides, having $\lambda \approx 1$.

The FP-LMTO calculations of the field-induced spin and orbital (Van Vleck) magnetic moments were carried out for YNi$_2$B$_2$C, LaNi$_2$B$_2$C, and LuNi$_2$B$_2$C compounds with inclusion of the Zeeman operator (1) in the external magnetic field $B = 10$ T. For the tetragonal crystal structure, the corresponding contributions to the magnetic susceptibility, $\chi_{\text{spin}}$ and $\chi_{\text{orb}}$, were calculated for the external field directed along the $c$ axis. The values of magnetic susceptibility $\chi_{\text{theor}} = \chi_{\text{spin}} + \chi_{\text{orb}}$ calculated for YNi$_2$B$_2$C, LaNi$_2$B$_2$C, and LuNi$_2$B$_2$C are listed in Table 2 in comparison with the available experimental data.

In the general form, the total magnetic susceptibility can be decomposed in the following terms (see Ref. [15]):

$$
\chi_{\text{tot}} = \chi_{\text{spin}} + \chi_{\text{orb}} + \chi_{\text{dia}} + \chi_{\text{L}},
$$

where present, respectively, Pauli’s spin susceptibility ($\chi_{\text{spin}}$), Van Vleck orbital paramagnetism ($\chi_{\text{orb}}$), Langevin diamagnetism of closed ion shells ($\chi_{\text{dia}}$), and the orbital diamagnetism of conduction electrons ($\chi_{\text{L}}$). It can be seen in Table 2 that the spin and orbital Van Vleck susceptibilities are the principal terms in Eq. (5). It is important that $\chi_{\text{orb}}$ gives a substantial contribution to the full paramagnetic susceptibility of borocarbides. The theoretical calculation of the Landau diamagnetism $\chi_{\text{L}}$ for the multiband dispersion law $E(k)$ represents a very difficult task [15]. However, a good fit of the experimental susceptibilities of YNi$_2$B$_2$C and LuNi$_2$B$_2$C with the calculated paramagnetic contributions to $\chi$ (see Table 2) indicates that, in these superconducting systems, the diamagnetic contributions in (5) are insignificant.

### 2.2. $R$Fe$_4$Al$_8$

Compounds $R$Fe$_4$Al$_8$ possess the body-centered tetragonal crystal structure of the ThMn$_12$-type, which belongs to the $I4/mmm$ space symmetry group [26]. In case of non-magnetic trivalent transition metals ($R = Sc, Y, Lu$), the AFM ordering of iron moments was established in $R$Fe$_4$Al$_8$ at low temperatures, though there are very inconsistent experimental data in the literature about a character of AFM ordering, ordering temperatures, and magnetic moments (see [2, 26–28] and references therein).

Virtually, no band structure calculations have been carried out to date for $R$Fe$_4$Al$_8$. In work [27], the main attention was paid to calculations of the iron magnetic moments in the magnetically ordered phases of $Y$Fe$_4$Al$_8$. In the present work, the DFT electronic calculations are carried out for $Y$Fe$_4$Al$_8$, ScFe$_4$Al$_8$, and LuFe$_4$Al$_8$ compounds in the paramagnetic, ferromagnetic (FM), and antiferromagnetic (AFM) phases.

The calculated DOS of the paramagnetic phase of LuFe$_4$Al$_8$ is presented in Fig. 3. The densities

### Table 1. Thermodynamic properties of $R$Ni$_2$B$_2$C borocarbides ($R$=Y, La, Lu).

| Combination | $V$, Å$^3$ | $N(E_F)$, states/eV·cell | $\gamma$ (exp), mJ/mol·K$^2$ | $\Theta_D$, K | $\lambda$ | $T_c$(exp), K | $T_c$(theor), K |
|-------------|---------|-----------------|----------------|---------|---------|---------|---------|
| YNi$_2$B$_2$C | 65.9 | 4.30 | 18.2 | 490 | 0.8 | 15.6 | 15.3 |
| LaNi$_2$B$_2$C | 70.7 | 2.24 | 8.4 | 495 | 0.6 | — | 6.5 |
| LuNi$_2$B$_2$C | 63.8 | 4.07 | 19.5 | 360 | 1.0 | 16.6 | 17.8 |

### Table 2. Magnetic susceptibility of $R$Ni$_2$B$_2$C ($R$=Y, La, Lu).

| Compound | $x_{\text{spin}}$ | $x_{\text{orb}}$ | $x_{\text{theor}}$ | $x_{\text{exp}}$ |
|----------|-----------------|----------------|-----------------|----------------|
| YNi$_2$B$_2$C | 1.35 | 0.87 | 2.22 | 2.0 [24] |
| LaNi$_2$B$_2$C | 0.96 | 0.72 | 1.68 | 1.0 [24] |
| LuNi$_2$B$_2$C | 1.29 | 0.73 | 2.02 | 1.9 [25] |
of states \( N(E) \) for the isoelectronic ScFe\(_4\)Al\(_8\) and YFe\(_4\)Al\(_8\) compounds are very similar, and they differ in small details only. The calculated densities of states at the Fermi level are listed in Table 3, and the dominating contributions to \( N(E_F) \) come from the \( d \)-states of iron. As is seen from Fig. 3, the Fermi level for the PM phase of LuFe\(_4\)Al\(_8\) is located at the steep slope of the density of states, where \( N(E) \) quickly grows with the energy in the immediate proximity (~0.01 eV) to the sharp peak of DOS.

The peak of \( N(E) \) in Fig. 3 is split at the AFM ordering for spin-up and spin-down states, and this provides the formation of the magnetic moments on the iron atom. As is seen from Table 3, it is accompanied by a noticeable decrease in \( N(E_F) \) for the ferromagnetic and antiferromagnetic phases of RFe\(_4\)Al\(_8\). The distinction between the magnetic moments on a Fe atom for the FM and AFM phases appeared insignificant in the case of LuFe\(_4\)Al\(_8\) and more noticeable in ScFe\(_4\)Al\(_8\). For all three investigated RFe\(_4\)Al\(_8\) compounds, the minimum of the total energy is found for the AFM ordering of the Fe moments in the basal plane along the [100] type directions. The calculated values of magnetic moments from Table 3 are qualitatively consistent with the experiments of Ref. [28] for LuFe\(_4\)Al\(_8\) \((\approx 1.3\mu_\text{B})\) and the results of calculations in [27] for YFe\(_4\)Al\(_8\) \((\approx 1.25\mu_\text{B})\).

The calculated value of DOS at the Fermi level for the AFM phase of LuFe\(_4\)Al\(_8\), \( N(E_F) = 14.3 \) states/(eV·cell), can be compared with experimental data on the electronic specific heat coefficient in this compound, \( \gamma_{\text{exp}} = 70 \) mJ/mol·K\(^2\) [2]. According to (2), the corresponding renormalization parameter for effective masses is about \( \lambda \approx 1 \), which is qualitatively consistent with the observation of superconductivity in LuFe\(_4\)Al\(_8\) [2]. It is necessary to consider, however, a contribution of the spin-fluctuation term in (4), which can be rather large for systems with high values of \( N(E_F) \), to \( \lambda \) [15]. Therefore, the question remains open: Can spin-fluctuations affect superconductivity in RFe\(_4\)Al\(_8\) compounds and, if so, how?

2.3. \textit{FeSe}

The calculations of the electronic structure of FeSe were performed for the tetragonal \( P4/mmm \) structure and for the orthorhombic \( Cmma \) structure, which correspond to the non-magnetic superconducting phase. The crystal lattice parameters of FeSe were taken according to data of Refs. [3, 4, 29, 30]. The calculated density of electronic states of the tetragonal FeSe is presented in Fig. 4, where the dominating contribution to \( N(E_F) \) comes from the 3d-states of iron.

As is seen in Fig. 4, the Fermi level is located in a close proximity (~0.1 eV) to the sharp peak of the density of electronic states. A similar feature of \( N(E) \) near \( E_F \) appears also in the orthorhombic phase of FeSe. It should be noted that fine details of the electronic spectrum, in particular, positions of the critical points of \( E(k) \) relatively to \( E_F \), can be reliably determined by the \textit{ab initio} calculations within DFT with an accuracy no more than 0.1 eV.

According to the results of calculations of the electronic structure and the magnetic susceptibility in the normal state in an external magnetic field, FeSe com-

---

**Fig. 3.** Density of electronic states \( N(E) \) of LuFe\(_4\)Al\(_8\) in the paramagnetic phase. The Fermi level \( (E = 0) \) is marked by the vertical line.

**Table 3.** Densities of electronic states at the Fermi level and the magnetic moments of iron atoms for RFe\(_4\)Al\(_8\) compounds \((R = \text{Sc, Y, Lu})\) in the paramagnetic (PM), ferromagnetic (FM) and antiferromagnetic (AFM) phases.

| Combination | \( N(E_F) \) states/(eV·cell) | \( M \) \( \mu_\text{B} \) |
|------------|------------------------------|-----------------|
|            | PM  | FM  | AFM | FM  | AFM |
| ScFe\(_4\)Al\(_8\) | 25.2 | 10.5 | 14.5 | 1.20 | 1.17 |
| YFe\(_4\)Al\(_8\) | 26.5 | 8.4  | 14.7 | 1.27 | 1.25 |
| LuFe\(_4\)Al\(_8\) | 27.0 | 11.5 | 14.3 | 1.24 | 1.22 |
pound is very close to a magnetic instability with the dominating exchange-enhanced spin paramagnetism \(\chi_{\text{spin}}\). Within the Stoner model, the exchange-enhanced Pauli spin contribution to the magnetic susceptibility can be presented as 
\[
\chi_{\text{spin}} = S \mu_B^2 N(E_F),
\]
where \(S\) is the Stoner factor, \(N(E_F)\) is the density of states at the Fermi level, \(\mu_B\) is the Bohr magneton. The calculated value of DOS at the Fermi level for FeSe amounts to \(N(E_F) \approx 1\) states/(eV-cell), allowing a small uncertainty in the determination of lattice parameters. Using the experimental value of susceptibility of FeSe at low temperatures, \(\chi \approx 1.6 \times 10^{-4}\) emu/mol [31], we obtained the Stoner factor \(S \approx 5\).

The calculated \(N(E_F)\) can be compared with experimental data on the electronic specific heat coefficient in FeSe, \(\gamma_{\text{exp}} = 5.73\) mJ/mol·K² [32]. According to (2), the corresponding parameter of renormalization of the effective masses amounts to \(\lambda \approx 1.4\). Assuming the validity of formalism (3) for the superconducting transition in FeSe at 8 K and using the experimental value \(\Theta_D = 210\) K from [32], it is possible to estimate the corresponding electron-phonon interaction parameter, \(\lambda_{\text{el-ph}} \approx 0.9\). However, it is necessary to consider also the spin-fluctuation term, according to (4), which gives \(\lambda_{\text{sf}} \approx 0.5\).

The experimentally observed large effects of a pressure on the superconducting transition temperature [3, 4] and on the magnetic susceptibility [31] gave evidence of substantial changes in the electronic structure of FeSe under pressure. In order to clarify a nature of these changes, the geometry optimization was performed for the tetragonal \(P4/nmm\) structure of FeSe within the GGA approach [19] and Elk program [17]. In such a way, the pressure dependences of the crystal lattice parameters were calculated. In particular, a growth of the relative height \(Z\) of selenium atoms over the iron atoms plane under applied pressure was established. These results are in a qualitative agreement with experimental data of Refs. [29, 30].

With the use of the established dependences of lattice parameters of FeSe under pressure, we have calculated the corresponding behavior of DOS at the Fermi level, \(N(E_F, P)\), which is presented in Fig. 5. It should be noted that the value of \(N(E_F, P = 0)\) calculated within the GGA approach is by \(~1.5\) times larger than the corresponding value in Fig. 4, which was calculated in the LDA approach [18]. For the

\[\begin{align*}
\text{Fig. 4.} & \quad \text{Density of electronic states } N(E) \text{ of FeSe. The Fermi level } (E = 0) \text{ is marked by the vertical line.} \\
\text{Fig. 5.} & \quad \text{Pressure dependence of the density of electronic states of FeSe at the Fermi level, } N(E_F). \text{ The inset shows the pressure dependence of the superconducting transition temperature for FeSe taken from Ref. [5].}
\end{align*}\]
perconductivity, or an alternative mechanism, which could involve, in a similar fashion, the density of electronic states at the Fermi level.

3. Conclusions

The calculations of the densities of electronic states of \( RNi_2B_2C \), \( RFe_4Al_8 \), and \( FeSe \) compounds indicate that the Fermi energy in these systems is located in a vicinity of the pronounced peaks in \( N(E) \). This confirms the recent ARPES observations that the proximity of Van Hove spectral features to the Fermi level can be considered as a key component for a realization of the superconductivity in transition metal compounds [10]. Though the main contribution to DOS for all three systems in a vicinity of \( E_F \) comes from the quasi-two-dimensional layers of 3d-metal atoms, nickel and iron, the \( N(E) \) dependences appear to be notably different. The Fermi level in \( RFe_4Al_8 \) is located just at the peak of \( N(E) \) and in the area of high values of DOS. As for \( RNi_2B_2C \) and \( FeSe \) compounds, the Fermi level is actually in the “pseudo-gap” area of electronic spectra with rather low values of \( N(E_F) \).

The results of calculations of the electronic structure allow us to analyze the experimental data on the electronic specific heat coefficient (in \( RNi_2B_2C \), \( LuFe_4Al_8 \), \( FeSe \)) and the cyclotron masses (DHVA effect in \( YNi_2B_2C \) and \( LuNi_2B_2C \)). The estimated renormalization parameters of the effective mass of conduction electrons indicate a possibility to realize the electron-phonon mechanism of superconductivity in these systems with \( \lambda_{el-ph} \approx 1 \). Along with this, the estimates indicate a noticeable contribution of the electron-paramagnon (spin-fluctuation) interactions to \( \lambda \), which complies with a proximity of \( RNi_2B_2C \), \( RFe_4Al_8 \) and \( FeSe \) to the magnetic ordering.

It is shown that the available experimental data on the strong pressure dependence of the magnetic susceptibility and the superconducting transition temperature in \( FeSe \) are caused by an increase in the density of electronic states at the Fermi level under pressure. The experimentally established nonmonotonic dependence of the superconducting transition temperature on the pressure in \( FeSe \) qualitatively correlates with the calculated behavior of DOS at the Fermi level in a wide range of pressures (Fig. 5).

This work was supported by the Russian-Ukrainian RFBR-NASU project 01-02-12.

1. K.-H. M"uller, M. Schneider, G. Fuchs, and S.-L. Drechsler, in: *Handbook on the Physics and Chemistry of Rare Earths*, edited by K.A. Gschneider, jr., J.-C.G. B"unzli, and V.K. Pecharsky (Elsevier, Amsterdam, 2008), p. 175.
2. V.M. Dmitriev, N.N. Prentslau, I.V. Zolotchevskii, L.A. Ishchenko, A.V. Terekhov, B.Ya. Kotur, W. Suski, and E. Talik, Low Temp. Phys. 29, 901 (2003).
3. Y. Mizuguchi and Y. Takano, J. Phys. Soc. Jpn. 79, 102001 (2010).
4. J. Wen, G. Xu, G. Gu, J.M. Tranquada, and R.J. Birgeneau, Rep. Progr. Phys. 74, 124503 (2011).
5. M. Bendele, A. Icshanow, Yu. Pavshchevich, L. Keller, Th. Strassle, A. Gusev, E. Ponomarkushina, K. Conder, R. Khasanov, and H. Keller, Phys. Rev. B 85, 064517 (2012).
6. M. Divis, K. Schwarz, P. Blaha, G. Hilscher, H. Michor, and S. Khmelevskyi, Phys. Rev. B 62, 6774 (2000).
7. A.O. Shorikov, V.I. Anisimov, and M. Sigrist, J. Phys.: Condens. Matter 18, 5973 (2006).
8. A. Subedi, L. Zhang, D.J. Singh, and M.H. Du, Phys. Rev. B 78, 134514 (2008).
9. K.-W. Lee, V. Pardo, and W.E. Pickett, Phys. Rev. B 78, 174502 (2008).
10. A.A. Kordyuk, Low Temp. Phys. 38, 901 (2012).
11. G. Goll, M. Heinecke, A.G.M. Jansen, W. Joss, L. Nguyen, E. Steep, K. Winzer, and P. Wyder, Phys. Rev. B 53, R8871 (1996).
12. B. Bergk and J. Wosnitza, Low Temp. Phys. 35, 687 (2009).
13. T. Baba, T. Yokoya, S. Tsuda, T. Watanabe, M. Nohara, H. Takagi, T. Oguchi, and S. Shin, Phys. Rev. B 81, 180509(R) (2010).
14. J. Maletz, V.B. Zabolotnyy, D.V. Evtushinsky, S. Thirupathaiah, A.U.B. Walter, L. Harnagea, A.N. Yaresko, A.N. Vasiliev, D.A. Chareev, E.D.L. Rikken, B. B"uchner, and S.V. Borisenko, arXiv:1307.1280 [cond-mat.supr-con] (2013).
15. G.E. Grechnev, Low Temp. Phys. 35, 638 (2009).
16. J.M. Wills, M. Alouani, P. Andersson, A. Delin, O. Eriksson, A. Grechnev, Full-Potential Electronic Structure Method. Energy and Force Calculations with Density Functional and Dynamical Mean Field Theory (Springer, Berlin, 2010).
17. http://elk.sourceforge.net/
18. U. von Barth and L. Hedlin, J. Phys. C: Solid State Phys. 5, 1629 (1972).
19. J.P. Perdew, K. Burke, and M. Ernzerhof, Phys. Rev. Lett. 77, 3865 (1996).
20. J.W. Lynn, S. Sthanakumar, Q. Huang, S.K. Sinha, Z. Hussain, L.C. Gupta, R. Nagarajan, and C. Godart, Phys. Rev. B 55, 6584 (1997).
21. H. Michor, T. Holubar, C. Dusek, and G. Hilscher, Phys. Rev. B 52, 16165 (1995).
22. D.R. Sanchez, S.L. Bud’ko, and E.M. Baggio-Saitovitch, J. Phys.: Condens. Matter 12, 9941 (2000).
23. W.L. McMillan, Phys. Rev. 167, 331 (1968).
Г.Є. Гречнєв, О.В. Логоша, А.О. Легенька, О.Г. Гречнєв, О.В. Федорченко

ЕЛЕКТРОННА СТРУКТУРА І ВЛАСТИВОСТІ НОВІТНИХ ШАРУВАТИХ НАДПРОВІДНИКІВ

Р е з ю м е

На основі теорії функціонала густини (DFT) проведено систематичне вивчення електронної енергетичної структури і магнітних властивостей шаруватих надпровідників $\text{RNi}_2\text{B}_2\text{C}$, $\text{RFe}_4\text{Al}_8$ і FeSe. Обчислення дозволили виявити ряд специфічних особливостей електронної структури, що можуть відповідати за незвичайні структурні, магнітні та надпровідні властивості цих систем. Продемонстровано, що енергія Фермі розташована в околі піків густини електронних станів (DOS). Головний внесок в DOS на рівні Фермі дають 3d-електрони. Обчислення ефектів тиску на електронну структуру і магнітну сприйнятливість у нормальному стані вказують, що в цих нових надпровідниках домінують спінові парамагнетизм і вони близькі до магнітної нестаабільності. Показано, що експериментальні дані по залежності надпровідного переходу в FeSe від тиску якісно кореляють з розрахованою поведінкою DOS на рівні Фермі під тиском.