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Sergei Kruchinin
National Academy of Sciences of Ukraine

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THE ELECTRONIC PROPERTIES OF NEW Fe-BASED SUPERCONDUCTORS

SERGEI P. KRUCHININ[1], VICTOR YA. ANTONCHENKO[1]
AND ARKADIY A. ZOLOTOVSKY[2]

[1] *Bogolyubov Institute for Theoretical Physics, NASU,*
Metrologicheskaya 14-b, Kiev 03143, Ukraine
skruchin@i.com.ua

[2] *Lashkaryov Institute of Semiconductor Physics,*
Prosp. Nauky 45, Kiev 03028, Ukraine

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Abstract: We investigate the band structure of Fe-based superconductors using the first-principle method of density-functional theory. We calculated the band structure and the density of states at the Fermi level for ReFeAsO (Re = Sm, Dy, Ho, Er) superconductors. Our calculations indicate that the maximum critical superconducting transition temperature T_c will be observed for compounds with Sm and Er. We predict that $T_c = 60\,\text{K}$ for ErFeAsO.

Keywords: Fe-based superconductors, band structure, density of states, critical superconducting transition temperatur

1. Introduction

The discovery of a new class of high-temperature superconductors – Fe-based layered compounds – aroused a significant interest at the beginning of 2008 gave hope for a progress in the synthesis of novel high-temperature superconductors (HTSC) up to room-temperature superconductors [1]. The nature of high-temperature superconductivity is not completely understood yet. The principal task of solid-state physics is the creation of superconductors which would ensure superconductivity at room temperature. Therefore, the large-scale search for such high-temperature superconductors is proceeding and intensified.

The crucial role in the explanation of physical properties of superconductors is played by calculations of the electronic structure from the first principles. It is worth noting that one of the basic properties of high-temperature superconductors is the presence of a lot of bands [2]. In work [3], it was shown that the formation of a superconducting state depends essentially on the density of states near the Fermi surface.

In the present work, we will investigate the band structure of some Fe-based compounds, by using the first-principle method of density-functional theory. Compound SmFeAsO showed the evidence of superconductivity at as high as 55K. This superconductor has a complicated multiband structure. We calculated the band structure and density of states at the Fermi level for ReFeAsO (Re = Sm, Dy, Ho, Er) superconductors.

Our calculations indicate that the maximum critical superconducting transition temperature T_c will be observed for compounds with Sm and Er. We predict that $T_c = 60$K for the hypothetical compound ErFeAsO.

2. Methodology

We calculate the band structures of HTSC, by using the BandLab program. This program is designed for Windows computer systems and performs calculations of the electronic structure of crystalline solids.

The bands are calculated using the method outlined by Pickett [4] within the density-functional scheme [5]. Since a summary of the method and its applications has been presented by Devreese and Van Camp [6], we outline the method here only in brief.

Starting with the N-electron problem in the field of ionic potentials

$$V_{\mathrm{ion}}(r) = \sum_m v_{ion}(r - R_m) \tag{1}$$

with the ions at static positions R_m, we have the Hamiltonian

$$H = \sum_i p_i^2/2m + \int n(r)V_{ion}(r)dr + \frac{1}{2}\iint n(r)v(r-r')n(r')drdr' \tag{2}$$

where, $n(r)$ is the electron density operator at r, and $v(r-r')$ is the Coulomb interaction. Hohenberg and Kohn established that there is a one-to-one correspondence between the ionic potential V_{ion} (to within an arbitrary constant) and the ground state density n, so that the many-body problem can be considered as a functional of the density, rather than a functional of the potential [4].

Hohenberg and Kohn [5] established that, for variations δn of the energy density which conserve the particle number N, the ground-state energy functional $E[n]$ is minimized by the ground-state density, with corrections of the order of δn^2. The resulting variational principle allows one to accurately obtain numerical results.

The energy functional has the form:

$$E[n] = T_0[n] + \int V_{\mathrm{ion}}(r)n(r)dr + \frac{1}{2}\iint n(r)v(r-r')n(r')drdr' + E_{\mathrm{xc}}[n] \tag{3}$$

where $T_0[n]$ is the kinetic energy of the system of interacting electrons with the density $n(r)$, and $E_{\mathrm{xc}}[n]$ is the exchange-correlation energy. If one has adequate approximations for $T_0[n]$ and $E_{\mathrm{xc}}[n]$, the energy can be obtained directly from relation (3), by the minimization with respect to $n(r)$. The energy functional is minimized by the density functional described by the above-presented relations, by performing iterations to attain the self-consistency.

Within the density-functional theory, the one-electron eigenvalues and eigenfunctions have no physical meaning and are not physically realizable. Some reviews containing discussions of applications of the density-functional theory, as well as the generalization to spin-polarized systems, are given, for example, in [7].

3. Band structures of a number of oxypnictides ReOFeAs

The crystal structure of compound LaOFeAs is shown in Figure 1. Such substances possess the tetragonal structure at room temperature. The crystal structure is formed by alternating FeAs layers revealing antiferromagnetism which are separated by LaO layers. The results of calculations of the electronic spectrum can be found in [8–11]. It should be emphasized that the specific features of the electronic spectrum are related to the quasi-two-dimensional character of superconductivity in FeAs planes.

In many works, an increase in T_c which is caused by the replacement of La by other rare-earth elements is frequently named the “chemical” pressure. A similar effect is characteristic of high-temperature superconductors [12]. The situation with the substitution of rare-earth elements in the series of compounds ReFeAsO is analogous to that in cuprate superconductors ReBaCuO. As distinct from cuprates, the substitution of various rare-earth ions into the series of compounds ReFeAsO leads to a quite large dispersion of values of T_c. It is possible to propose two explanations for the scenario of this phenomenon.

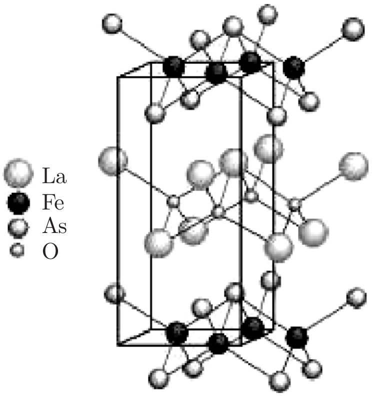

Figure 1. Crystalline structure of LaFeAsO

First, it can be caused by the effects of a disorder arising at the substitution of rare-earth elements, so that the anomalous pairing (*e.g.*, anisotropic pairing, d-pairing, *etc.*) is realized in FeAs. Second, we may consider the magnetic mechanism of pairing in Fe-based superconductors.

Spins of rare-earth ions interact strongly with spins of iron and can essentially influence the spectrum of spin fluctuations in FeAs planes, which increases T_c if the magnetic mechanism of pairing is dominant.

We have carried out *ab initio* calculations for a number of oxyphictides ReFeAsO in the framework of an approach based on density-functional theory. The results of calculations are presented in Figures 2–4 for the band structure and the density of states in ReFeAsO. At a comprehensive study of the density of states, the relationship of the density of states at the Fermi level and the value of T_c is revealed. In Figure 5, we give the dependence of T_c on the density of states $N(E_f)$ on the Fermi surface. In the calculations of T_c, we used the Bardeen-Cooper-Schrieffer formula:

$$T_C = 1.14\frac{\theta}{k_B}\exp\left(-\frac{1}{N(E_f)V}\right) \tag{4}$$

where θ – Debye energy, V – attractive pairing potential acting between electrons, $N(E_f)$ – density of state on the Fermi surface.

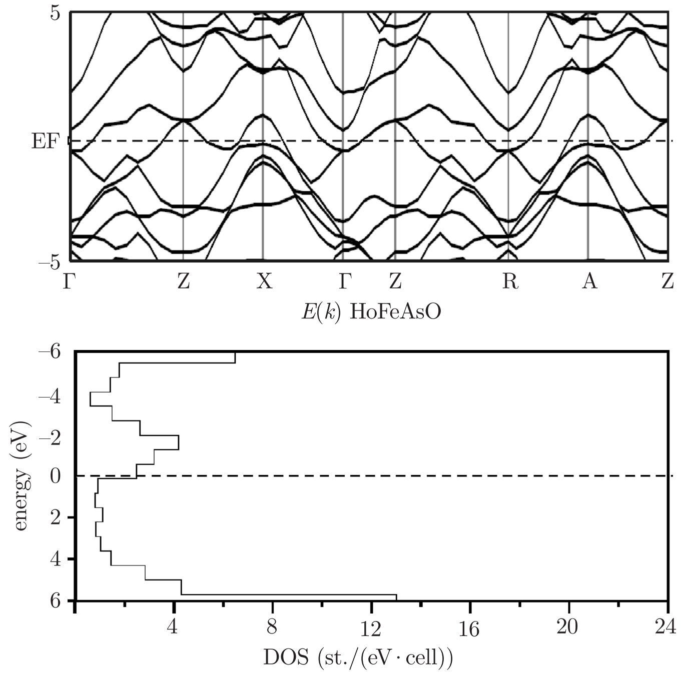

Figure 2. Results of our calculations of the band structure and the density of states for HoFeAsO with $T_c = 50.3$K

4. Summary

The discovery of a new type of high-temperature superconductivity in FeAs generates the expectation of the appearance of novel superconductors with higher T_c by means of the doping that consists in the substitution of the atoms lying

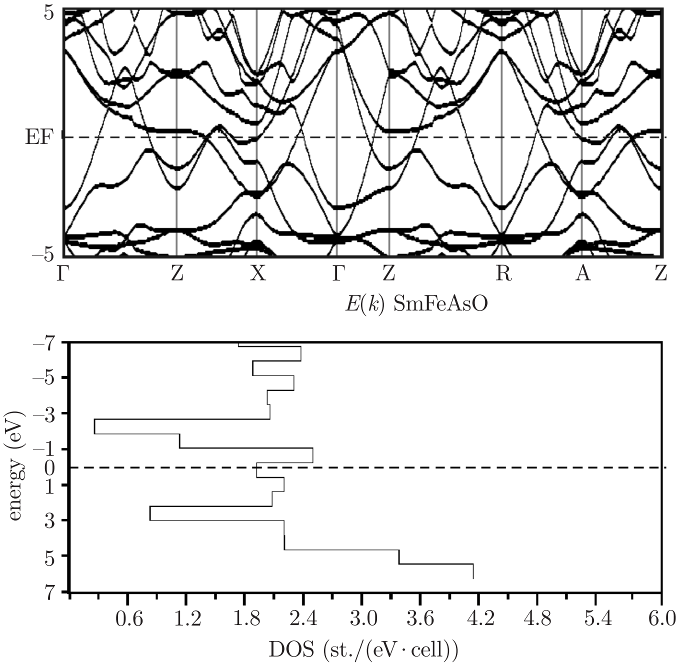

Figure 3. Results of our calculations of the band structure and the density of states for SmFeAsO with $T_c = 55.0$K

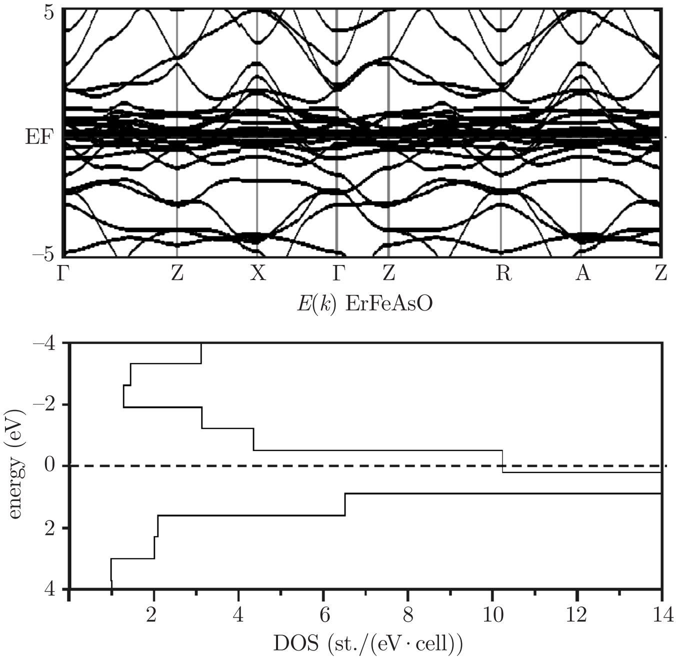

Figure 4. Results of our calculations of the band structure and the density of states for ErFeAsO

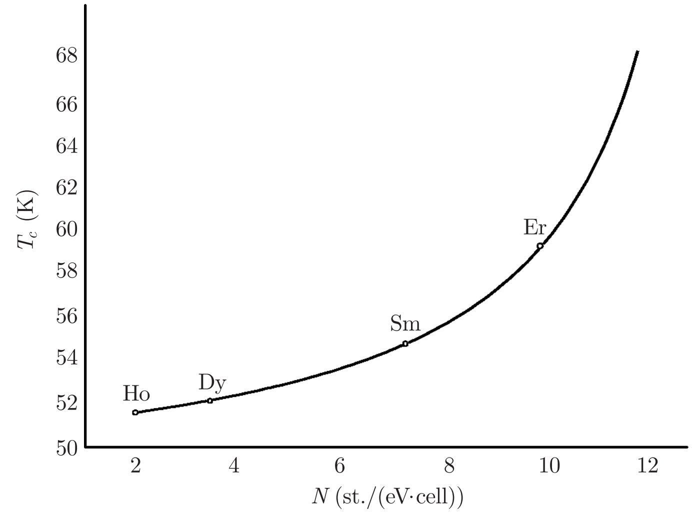

Figure 5. Dependence of T_c on the density of states on the Fermi surface $N(E_f)$ for ReFeAsO

outside of the principal layers of compound FeAs. In FeAs, the possibilities to dope are high due to the easy replacement of chemical elements. In compounds ReFeAsO, the substitution of the rare-earth element is of special interest. We have carried out the *ab initio* calculations for a number of oxypnictides ReOFeAsO in the framework of density-functional theory. Out results indicate that the maximum critical superconducting transition temperature T_c will be attained for compounds with Sm and Er. Our prediction is $T_c = 60$K for ErFeAsO.

Acknowledgements

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