Pis'ma v ZhETF, vol. 111, iss. 4, pp. 228 – 229

Electronic structure of transition-metal pnictides oxides $La_3T_4As_4O_2$ phase (T = Ni, Cu) from *ab-initio* calculations

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Submitted 2 November 2019
Resubmitted 2 November 2019
Accepted 9 January 2020

DOI: 10.31857/S0370274X20040049

Oxypnictide systems based on transition metals and rare earths offer a promising platform to understand the physical properties of the new superconducting pnictide compounds [1, 2]. The family 3442-type $Ln_3T_4Pn_4O_2$ is one of the oxypnictide phases that interest us particularly. A number of experimental research studies have been published for this type of compounds [3–9] but just a few theoretical studies *ab-initio* have been reported [3, 10]. Their crystalline structure represents a convolution of the structure of the families 122 [11, 12] and 1111 [13] of pnictides. The lanthanum compounds reported in [9] in the two T = Cu, Ni series show a Pauli paramagnetic behavior and a $T_C = 1.7\,K$ superconductivity was reported only in the $La_3Ni_4As_4O_{2-\delta}$ compound. None of the others compounds synthesized in [9] is superconducting, however, a complex magnetic behavior is observed. $Ce_3Cu_4As_4O_{2-\delta}$ is the only nonmetal among all the compounds presented. Note that the superconductivity was also observed at low critical temperature $T_C = 2.2\,K$ previously in the analogous compound $La_3Ni_4P_4O_2$ [3]. Very few *ab-initio* calculations on this series of 3442-compounds have been reported so far to our knowledge [3, 10].

In this work, we have chosen to determine the structural and electronic properties of the new $La_3T_4As_4O_2$ compounds with a lamellar structure, based on lanthanum and arsenic for T = Ni, Cu, in order to contribute to a better exploration and knowledge of these compounds. Property calculations were also made for the quaternary and ternary compounds LaTAsO and LaT_2As_2 (T = Ni, Cu). Finding points in common between the three families makes it possible to identify certain criteria that might favor superconductivity at higher temperatures in these compounds.

We employ the hybrid full-potential augmented plane wave plus local orbital method within the density functional theory as implemented in WIEN2k code [14]. We perform calculation of electronic structure of $La_3T_4As_4O_2$ (T = Ni, Cu) compounds using the local density approximation LDA [15], the generalized gradient approximation GGA [16] together with their onsite Coulomb interaction added versions, LDA + U and GGA + U [17].

First, we investigated the electronic structure of $La_3T_4As_4O_2$ (T = Ni, Cu) by the first principle calculations. We also studied the electronic structure of the 1111 and 122 systems because they would be of great help for better understanding the physical properties of the 3442 materials. The absence in literature of any information about the *ab-initio* electronic structure of the 3442-compounds leads us to study these new materials, which offer a new voice towards the superconductivity. For this, we have used four different approaches in order to give a better description of the electronic structure of the studied systems. Effectively, the GGA calculations give correct ground state properties comparing favorably with their similar P-3442 compound [3] and the synthesized 3442 systems with vacancies [9]. All structural parameters such as lattice constants, internal parameters, interatomic distances and angles are comparable to experimental [11] (3442 structures with vacancies) and theoretical [3] (P-3442) data. We note that the lattice constants (a_0 and c_0) satisfy the inter-growth conditions of the "3442" structure. The band structure and the density of states of $La_3Ni_4As_4O_2$ compound are found very comparable with the results of I. R. Shein and A. L. Ivanovskii [3] for $La_3Ni_4P_4O_2$ compound. We found a topological similarity between the Fermi surfaces of Ni-3442 and Ni-1111 systems, which respect the five band model. We strongly believe that this range of materials can be a promising platform for new su-

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perconducting properties and oxygen vacancies in 3442-structures will be our perspective for future *ab-initio* predictions of new superconductors.

Full text of the paper is published in JETP Letters journal. DOI: 10.1134/S0021364020040013

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