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Title: **Investigation of the electronic structure of intermetallic compounds with linear Dirac/Weyl dispersion of bands**

Abstract of the doctoral thesis

The discovery of the quantum Hall effect and then graphene, insulators and topological semimetals in the last few decades has resulted in a paradigm change in the description of crystalline systems and their electronic structure. The consequence of this pioneering research is the search for new systems with non-trivial band structure topology which is now a leading area of solid state physics. Topological semimetals are three-dimensional materials, in whose electronic structure energy bands of linear dispersion are present, forming characteristic Dirac or Weyl-type conical structures. These three-dimensional analogs of graphene were originally detected among systems that are a combination of *p*- and *d*-electron atoms, such as TaAs or Na_3Bi. The purpose of this doctoral dissertation, in the form of a series of 6 publications, was to investigate theoretically using computational methods *ab initio* the electronic structures of selected intermetallic compounds in terms of the presence of Dirac- or Weyl-type states in them and their potential influence on transport properties. In four of the publications of the series, electronic structures (including band dispersions, densities of states and Fermi surfaces) were determined and their properties were studied for selected compounds belonging to the 112 family (La;Ce)M(As;Sb;Bi)$_2$, where M is a transition metal element. In the band structure of La(Ni;Cu;Pd)Sb_2 superconductors, Dirac-like bands, inherent to systems with a square net composed of *p* block atoms, were detected. The associated Dirac fermion quasiparticles may be responsible for the superconductivity of these compounds. In addition, the dependence of the critical temperature values of these superconductors on the dimensionality of the Fermi surface sheets under the Feshbach resonance scenario of its shape was noticed. On the other hand, the $CeAgAs_2$ antiferromagnet has been comprehensively investigated by means of various experimental methods, and then the results of which have been interpreted based on the theoretically determined electronic structure of the magnetically ordered state. In this compound, two distinct groups of electronic states related to the cis–trans transition in the absence of Dirac-type bands were recognized, probably due to the distortion of the arsenic sub-lattice and the reduced symmetry of the unit cell. In addition, a close relationship is shown between the electronic structures and properties of the $LaSb_2$ superconductor and the square-net Dirac semimetal, $LaAgSb_2$, known from the literature. For both compounds, the occurrence of linear magnetoresistance was related to the presence of linear bands and in consequences of two-dimensional Dirac fermions at the Fermi level. The effect of structural disorder in the $LaZn_{1-x}Bi_2$ system on the

electron structure of a Dirac nodal-line semimetal was also investigated theoretically using the method of model supercells. The following publication of the series examines the compound $CaIr_2Ge_2$ as a representative of family 122, composed of p- and d-electron atoms. Original experimental (electron transport) and theoretical (electron structure) results were presented for it and analyzed for topologically non-trivial states due to the value of the topological invariant and the presence of a split anisotropic Dirac cone. In the next publication in the series, a theoretical study of a solid solution of 11 type compound, $La_{1-x}Tl_xN$, was carried out. The publication focused on the analysis of changes in the topological properties of the band structure of the system, depending on the thallium content. The topologically non-trivial nature of the semimetal for the content of $x = 0.25$ was demonstrated. The obtained results were compared to similar systems known in the literature – topological insulators and semimetals with cubic crystal structures.