Fe-based Heusler alloys - tailoring of band structure and magnetic properties.

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Heusler alloys have been the subject of intensive research for many years due to their interesting electronic and magnetic properties, as well as their potential applications [1]. The Heusler alloy group includes compounds exhibiting, among others, the magnetic shape memory effect, superconductors and heavy fermion behaviour. Very promising for application are half-metallic compounds. Determining the spin polarisation of ferromagnetic materials is a key factor in the search for materials potentially suitable for use in spintronics, as ferromagnets with high spin polarisation are required for the implementation of high-performance devices. Full spin polarisation of charge carriers can only be achieved in the limiting case of zero temperature and vanishing spin-orbit interactions. Since most Heusler compounds containing only 3d elements show no spin-orbit coupling, they are potential alloys exhibiting half-metallic character [2]. In the group of Heusler alloys (X_2YZ, X, Y-transition metal atom, Z-metalloids atom), covalent hybridisation between the lower energy d states of high-valent transition metal atoms X and the higher energy d states of low-valent transition metal Y leads to the formation of an energy gap for one spin direction at the Fermi level. If the electric current is perfectly spin-polarised in the material, this enables production of new magnetic field-controlled devices. This differs significantly from traditional devices powered by electric charge. In addition to stoichiometric Heusler compounds, four- and five-component Heusler alloys also exhibit interesting properties [3]. Previous studies on this group of alloys have shown that slight changes in the concentration of individual components lead to significant changes in the electronic and magnetic properties of the alloys under investigation [4,5]. Therefore, band structure calculations can be a useful tool for designing materials with desired properties.

The aim of the planned research is to determine the electronic structure and magnetic properties of selected four- and five-component systems based on iron of the type $Fe_2A_xB_{1-x}C_yD_{1-y}$ (A, B – transition metals, C, D – metalloids) covering inter alia some Heusler alloys based on Fe bcc. First principle spin-polarized calculations have been carried out using the Full Potential—Linearized Augmented Plane Waves with Local Orbitals (FP-LAPW+lo) method implemented in Wien2k code [6].

References:

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