Effect of Intercalation by 3d-Transition Metals on Structural, Electronic and Magnetic Properties of β-InSe Layered Crystal

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Recently, as a perspective layered crystals for the spintronics devices, the indium selenides doped by the transition metals have attracted great attraction since it possesses magnetic properties. Intercalation of these crystals by such impurities with unclosed *d*-shells, on the one hand, makes it possible to obtain the structures which differ significantly from artificial two-dimensional magnetic materials, such as the structures with the layers of magnetic and non-magnetic atoms. On the other hand, the essential changing of the magnetic properties of intercalated systems takes place. The authors of experimental works [1-3] showed that hexagonal β-InSe crystals intercalated with transition metal impurities (Mn, Fe, Co, Ni) exhibit the ferromagnetic order. According to experimental data [1,2], the introduction of impurity atoms by means of intercalation in a magnetic field leads to hysteresis loops which are typical for ferromagnetics. The values of the Curie temperature and the coercive force [1] are also obtained for the considered materials.

In this report, utilizing first-principles calculations within density-functional theory the electronic and magnetic properties of the β-InSe layered crystal doped with 3*d*-elements have been investigated. We studied the possible ways intercalation of magnetic 3*d*-elements of the different concentrations in indium selenide crystals. It is shown that the impurities of 3*d*-metals can enter both in the structure of the layers and in the van der Waals space forming the "covalent bridges".

We carried out the calculations of the band spectra, the partial density densities and the spatial distribution of the valence electron density for a β-InSe crystal with different concentrations of transition metal impurities (Mn, Ni, Co). The changes in the spin-polarized spectra and partial charge densities for spin subsystems in diluted by magnetic impurities indium selenides has been analyzed. It was founded that diamagnetic structures of β-InSe after intercalation with 3*d*-elements become magnetically ordered. The results indicate that all 3*d*-transition metals produce localized magnetic moments. The estimates for the magnetic moment and their dependence on the concentration of impurities are obtained. It is shown that the local magnetic moment for Mn is greater than that for Ni and Co atoms. The decreasing of the magnetic moment of the impurity atoms in the In-Se layered crystals in a result of their intercalation by the transition metal atoms is observed too. The nature of the ferromagnetic ordering in intercalated β-InSe crystals is determined due to the hybridization of the *d*-states of the impurity with the *p*-states of the chalcogen. The systematic study about electronic and magnetic properties of the β-InSe layered crystal intercalated with 3*d*-elements by first principles calculations have been also explained in the framework of the diagonal Green' functions method for the *s-d* Anderson's model.

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