First principles calculations of zinc blende superlattice surfaces and multilayers with ferromagnetic dopants

A. Wronka

Department of Solid State Physics University of Łódź
Pomorska 149/153, 90-236 Łódź, Poland

Investigating and synthezing of new spintronic materials has a great practical importance due their applications to future information technology and electronic devices. Among all proposed materials the most widely promising properties exhibit semiconductors have been made by doping magnetic ions (V, Cr, Mn, Fe, Co, and Ni) or preparing a hybrid structure of magnetic element with a semiconductor [1].

Half metallic (HM) random (diluted) and digital ferromagnetic dopants attract much interest as they have only one occupied set of spin density of states at the Fermi level, and thus should be capable of 100% polarized spin current injection in principle. It has been reported that the half metallicity of MnAs/AsGa digital alloys can be destroyed by Fe monolayers embedded in these materials [2].

In this paper, in order to understand of half-metallicity conditions of Fe/MnAs/ AsGa(001) digital alloy superlattices, we calculated electronic and magnetic properties of zinc blende multilayers in the different ab initio supercell geometries. The atomic structure model from the previous paper [2] is extended to consideration of the surface ferromagnetic metal monolayer in the slab approximation. The calculations are performed by means of the DFT method within the full-potential and APW+lo approach. This work presents detailed information about total and atom projected DOS's in the surface region of the investigated systems. Our interest was to look for common trends and differences in the electronic structures for different locations of Fe adatoms in the zinc blende digital alloy surfaces and multilayers.

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Name of the presenting author (poster): Andrzej Wronka
e-mail address: awronka@uni.lodz.pl
url : http://www.fic.uni.lodz.pl/~awronka