First principles calculations of zinc blende superlattices ferromagnetic compounds

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Technological advances in device micro- and nano-fabrication over the past decade has enabled a variety of novel heterojunction device structures to be made in various electronic and spintronic devices [1]. Among these, magnetic half-metallic multilayers, superconductor/normal metal junctions and diluted ferromagnetic heterostructures (DFH) exhibit a rich variety of features, with the potential for future generations of electronic devices with improved sensitivity and quality.

The modeling of such structures in a flexible and accurate way, with a predictive capability is a great theoretical challenge. In particular, Mn/GaAs digital alloys with Mn and GaAs layers grown alternately by molecular beam epitaxy (MBE) exhibit some magnetic properties such as Curie temperature and coercive field intensity different from those of the (Ga, Mn)As random alloys, adding more possibilities of this new class of ferromagnetic semiconductors for technological applications [2, 3]. Theoretical ab initio calculations of thin superlattices of zinc blende compounds (MnAs, CrAs and GaAs) were performed in the framework of Density Functional Theory (DFT) by several authors [4, 5].

We investigate the electronic and magnetic structure of zinc blende superlatices and multilayers Fe/MnAs/AsGa(0,0,1) and Mn/AsGa digital alloy in different ab initio supercells geometry. The calculations are performed by means the DFT method within the general gradient approximation (GGA) with ultrasoft pseudopotentials, plane-wave basis, spin GGA and non-collinear magnetism. The bulk, surface and interface magnetic and electronic properties like total energy, magnetization, energy bands and DOS of zinc blende superlattices and multilayers with the ferromagnetic compounds have been calculated and compared.

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[1] I. Žutiĉ, J. Fabian, and S. Das Sarma, Rev. Mod. Phys. **76** (2004) 323.
[2] G. Kioseoglou *et al.,* Appl. Phys. Lett. **80** (2002) 1150.
[3] Y. L. Soo *et al.*, Appl. Phys. Lett. **80** (2002) 2654.
[4] M.C. Qian *et al*., Phys. Rev. B **71** (2005) 012414.
[5] S. Sanvito, Phys.Rev. B **68** (2003) 054425.

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