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Electronic Structure of Noble Metal Impurities and Ferromagnetic Ordering in Semiconductors

O.V. Farberovich[1], A. Yaresko[2], K. Kikoin[3], and V. Fleurov[3]*

[1]Department of Physics, Ben-Gurion University, Beer-Sheva 84105, ISRAEL
[2]Max-Planck-Institut für Physik Komplexer Systeme, Nöthnitzer Str. 38, D-01187 Dresden, GERMANY
[3]School of Physics and Astronomy, Beverly and Raymond Sackler Faculty of Exact Sciences, Tel Aviv University, Tel Aviv 69978, ISRAEL

*Corresponding author: Victor Fleurov, e-mail: fleurov@post.tau.ac.il

A numerical method for calculation of the electronic structure of transition metal impurities in semiconductors based on the Green function technique is developed. The electronic structure of 3d impurity is calculated within the LDA+U version of density functional method, whereas the host electron Green function is calculated by using the linearized augmented plane wave expansion. The method is applied to the Cu impurity in GaP. The results of calculations are compared with those obtained within the supercell LDA procedure. It is shown that in the Green function approach Cu impurity has an unfilled 3d shell. This result paves a way to explanation of the magnetic order in dilute Ga1-x CuxP alloys.

We apply the microscopic model of indirect exchange interaction between transition metal impurities in dilute magnetic semiconductors [1] in order to explain the ferromagnetic ordering Ga1-x CuxP alloys. According to this model the hybridization of the impurity d-electrons with the free states above the Fermi level is mainly responsible for the exchange of electrons between the impurities, whereas the Hund rule for the electron occupation of the impurity d-shells makes its spin selective. The molecular field is calculated by considering large ensembles of Cu atoms and the Curie temperature T_C dependence on the concentration is found. This approach has been also applied analyze ferromagnetic superexchange in the intrinsic ferromagnets TiO2 doped, where no free carriers are observed. In this case the ferromagnetic order arises due to superexchange between complexes [oxygen vacancies + magnetic impurities], which are stabilized by charge transfer from vacancies to impurities. The Hund rule controls the superexchange via empty vacancy related levels so that it becomes possible only for the parallel orientations of impurity magnetic moments.

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BB07

Magnetic Anisotropies in (Ga, Mn)As/GaAs Superlattices with Different GaAs Spacer Thicknesses

Sunjae Chung[1], Sun-young Yea[1], Taehee Yoo[1], Sanghoon, Lee[1]*, X. Liu[2], and J. K. Furdyna[2]

[1]Physics Department, Korea University, Seoul 136-701, KOREA
[2]Physics Department, University of Notre Dame, Notre Dame, IN 46556, USA

*Corresponding author: Sanghoon, Lee, e-mail: slee3@korea.ac.kr

We have investigated the magnetic properties of GaMnAs/GaAs superlattices (SLs) with different GaAs spacer thicknesses, which are range from d = 0.8 *nm* to 3.9 *nm*. The hole concentration of SLs obtained from Hall effect measurement at room temperature showed clear dependence on the thickness of GaAs spacer. The hole concentrations systematically varies from 0.965×10^{20} cm^{-3} to 2.83×1020 cm^{-3} as spacer thickness increases. Such variation of hole concentration in GaMnAs/GaAs SL structures may due to the different strain originated from different thickness of GaAs space layers. Such strain-induced change of carrier concentration in multi-layered structure is often called as *"piezo-electric" effect*. [1] Since the magnetic anisotropy of GaMnAs-based systems are known to have strong dependence on the carrier concentration, the magnetic anisotropy of all samples in the series have been further investigated by using planar Hall effect measurements. The magnetic anisotropy of SLs obtained from angular dependent PHE indeed showed systematic change with spacer thickness. Specifically, the temperature, at which transition occurs from dominant cubic to dominant uniaxial anisotropy, increases with an increase of spacer thickness in the GaMnAs/GaAs SLs. The observed systematic dependences of hole concentration and the magnetic anisotropy provide a new handle for controlling magnetic properties in GaMnAs-based heterostructures.

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