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Electronic Structure of Noble Metal Impurities and Ferromagnetic Ordering in Semiconductors

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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 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 unoccupied 3d
shell. This result paves a way to explanation of the magnetic order in dilute Ga1−xCuxP 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 in 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 STCS
dependence on the concentration is found. This approach has been also applied analytically to ferromagnetic superlattices in
the intrinsic ferromagnets Fe0.2O2 doped, where no free carriers are observed. In this case the ferromagnetic order arises due to
superexchange between complex (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.

REFERENCES

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

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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
0.605×10^20 cm^-3 to 2.83×10^20 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 spacer 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 is known to have strong dependence on the carrier concentration, the magnetic anisotropy of all
samples in the series have been further investigated 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 tuning magnetic properties in GaMnAs-based heterostructures.

REFERENCES