III-V SEMICONDUCTOR QUANTUM DOTS WITH A MAGNETIC IMPURITY

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A single transition-metal impurity in a semiconductor quantum dot (QD) seems promising for spintronics and quantum information processing. The $sp-d$ exchange interaction between the magnetic ion and the carriers, well characterized in bulk diluted magnetic semiconductors, is strongly enhanced by quantum confinement leading to a zero-field splitting of the exciton [1]. The excitonic photoluminescence (PL) in Mn-doped CdTe/ZnTe self-assembled QDs was indeed found to split into six components [2]. More recently, a strikingly different zero-field splitting pattern of the PL has been reported [3] in Mn-doped InAs/GaAs QDs, which arises from the difference in the nature of the Mn impurity in II-VI and III-V semiconductors.

We present a theoretical model for the electronic structure of GaAs and InAs quantum dots (QDs) containing a single substitutional Mn impurity. The Mn impurity in these compounds is known to be a shallow acceptor in the configuation $d^5 + h$. Our model for the hole states is based on the Luttinger Hamiltonian and the Coulomb potential with a central cell correction that accounts for the observed binding energy in the bulk. The total binding energy as well as the exchange contribution are found to increase with decreasing QD size. The effect is more pronounced in spherical nanocrystals (NCs) than in lens-shaped self-assembled QDs, because of the highly anisotropic confinement in the latter. With an on-center impurity, NCs retain the bulk T_d symmetry and the ground state is a $j = 3/2$ - like Γ_8 level. In self-assembled QDs it splits into two doublets: $\Gamma_6(|j_z| = 1/2)$ and $\Gamma_7(|j_z| = 3/2)$ of D_{2d}, which mix in the presence of in-plane asymmetry, both belonging to Γ_5 of the reduced symmetry C_{2v}. The order and the splitting between the doublets depend on the degree of confinement and the strain-induced separation between the light- and heavy-hole bands. In lattice-matched GaAs/(Ga,Al)As QDs the ground-state doublet is $|j_z| = 3/2$ - like in the low-confinement limit; as the QD size decreases there is a rapid cross-over to a $|j_z| = 1/2$ - like ground state in QDs of typical sizes. On the other hand, in strained InAs/GaAs QDs the ground state is always $|j_z| = 3/2$ - like and the splitting relatively large. The exchange coupling with the Mn spin $S = 5/2$ finally leads to a set of doubly degenerate energy levels, rather close to one another. Our results invalidate the previously adopted perturbative picture based on the bulk level scheme. We also study the lowest two-hole states: The ground state is a singlet almost uncoupled to the Mn spin. We deduce the zero-field fine structure of the excitonic transitions and compare our results with the experimental photoluminescence spectra [3] in Mn-doped InAs/GaAs QDs.

[1] A. K. Bhattacharjee and J. Pérez-Conde, Phys. Rev. B **68**, 045303 (2003); A. K. Bhattacharjee, *ibid.* **76**, 075305 (2007).
[2] L. Besombes *et al.*, Phys. Rev. Lett. **93**, 207403 (2004).
[3] A. Kudelski *et al.*, Phys. Rev. Lett. **99**, 247209 (2007).