Poster

Nanocrystals of Mn-doped CdTe: A theoretical approach on magnetic properties

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Progress in materials chemical synthesis, computational capabilities and scanning-probe techniques has permitted a detailed understanding of semiconductor nanocrystals, also referred to as quantum dots (QD's). Their properties are unusual at the macroscale, strongly dependent on size [1,2], doping [3-6] and shape [7]. In particular, Mn-doped II-VI nanocrystals, succesfully synthesized and characterized during the last fifteen years [3-6,8-13], show remarkable magneto-optical effects. Their interesting physical properties arise from strong *sp-d* exchange interactions between manganese impurities and band-edge states.

In this work we investigate the magnetic properties of Mn-doped CdTe nanocrystals in the frame of the density-functional theory, by means of the projector augmented-wave method. Mn impurities replace Cd atoms in the zinc blende lattice. When a single manganese atom is embedded, the calculated total magnetic moment associated with the quantum dot is $\mu_{QD} = 5\ \mu_B$, but the local moment on the manganese site is found to be smaller: $\mu_{Mn} = 4.65\ \mu_B$. This effect is attributed to the *sp-d* hybridization, which is also responsible for the appearance of small local moments on the manganese nearest neighbor tellurium atoms, which also contribute to the total moment μ_{QD}. When two impurities are included, we study two magnetic configurations, which correspond to the Mn moments initially parallel ($\mu_{QD} = 10\ \mu_B$) and antiparallel ($\mu_{QD} = 0\ \mu_B$). We find that the latter is the ground state. For the same reason than before, the calculated Mn local moments are found to be smaller in modulus than 5 μ_B. We also analyze the excited states μ^*_{QD} = 10, 0, 2, -2, 8 and 12 μ_B (a star stands for "excited"). In the excited ground state the Mn local moments are parallel with a total magnetic moment 10 μ_B. The differences in the magnetic behavior between the non-excited (antiparallel Mn moments) and the excited ground states can be attributed to a hole-mediated exchange interaction between the Mn magnetic moments. The derived *sp*-band-Mn-*d* and Mn-Mn exchange constants present smaller values than in bulk diluted magnetic semiconductors [14]. Nanocrystals with an extra electron, i.e. charged quantum dots, are also considered.

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