Electronic Structure and Magnetic Properties of Mn-doped CdTe Quantum Dots from First-Principles

C. Echeverría-Arrondo[1], A. Ayuela[2], J. Pérez-Conde[1], A.K. Bhattacharjee[3]
[1]Depto. de Física, Universidad Pública de Navarra, campus Arrosadía, s/n., Pamplona, Spain
[2]Donostia International Physics Center, Paseo Manuel de Lardizábal, 4, San Sebastián, Spain
[3]Laboratoire de Physique des Solides, UMR du CNRS, Université Paris-Sud, Orsay, France
carlos.echeverria@unavarra.es

Progress in materials chemical synthesis, computational capabilities and scanning-probe techniques has permitted a detailed understanding of semiconductor nanocrystals (NCs), also referred to as quantum dots (QDs). Their properties, unusual at the macroscale, are strongly dependent on size [1,2], doping [3-6] and shape [7]. In particular, Mn-doped II-VI NCs., successfully synthesized and characterized during the last fifteen years [3-6,8-13], are current research materials for new spin-based devices [14]. Most of their interesting properties arise from the exchange interaction between the Mn local moments and *sp* band states (either electrons or holes) [15,16], which results in a giant internal magnetic field [17,18] that splits the conduction- and valence-band edges [16]. This remarkable effect can be experimentally detected using microspectroscopy [11].

In this work we calculate the total energy of spin-polarized CdTe:Mn NCs by means of the projector augmented-wave method implemented in the VASP code. The considered dots contain Mn^{2+} impurities which replace Cd atoms in the lattice. When a single Mn atom is embedded, the total magnetic moment of the dot is 5 μ_B, as expected, but the Mn^{2+} local moment is found to be reduced to ~4.65 μ_B. This reduction is attributed to the *p-d* hybridization [15], which is also responsible for the appearance of small local moments on the non-magnetic neighbor sites (Te) [15]. When two Mn^{2+} impurities are included, the total magnetic moment of the dot is either 10 μ_B or 0 μ_B, depending on the previous magnetic configuration of the introduced Mn spins. In this case, the Mn^{2+} local magnetic moments are lower than 5 μ_B (in modulus), for the same reason than before. We calculate the total energy as a function of the impurities positions and the magnetic configuration, and we obtain the *sp-d* and *d-d* exchange constants $N_0\alpha$, $N_0\beta$ and J^{dd} [16]. We also study the effect of injecting an extra electron, in the most stable magnetic configuration of the dot containing two Mn^{2+} ions [19].

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