Ab initio studies of magnetic anisotropy energy in highly Co-doped ZnO

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ZnO is well known and intensively investigated wide-gap semiconductor with the wurtzite-type crystal structure. Both the transition-metal doped thin layers and bulk crystals of this compound or diluted magnetic semiconductors (DMS) grown on the basis of ZnO attract still a lot of attention due to continuous interest in materials for possible future applications in the area of spintronics. In particular, the Co-doped ZnO crystals exhibit interesting magnetic properties and have been the topic of several recent papers.

The aim of the present work is the theoretical analysis of the magnetic anisotropy energy (MAE) for a semiconductor with the wurtzite structure: ZnO crystal containing Co impurities. In the paper we discuss the results of extensive ab initio calculations of the MAE for 2x2x2 ZnO supercell containing 32 atoms with one Zn ion replaced by the Co ion. It is demonstrated that the effect of spin polarization of the surrounding atoms caused by the Co ion is almost limited to the four nearest oxygen neigbours only. As it could be expected, the influence of the Zn and O spin-orbit coupling on the MAE magnitude is very weak and one may claim that the magnetic anisotropy of Co is a single ion type anisotropy. On the contrary, the MAE is extremely sensitive to the lattice geometry and to the nearest neighbourhood of Co ion. For the ZnO lattice parameters the direction of magnetization easy axis is well reproduced. However, there exists a significant discrepancy between experimental and theoretical MAE value**,** the latter one is nearly order of magnitude smaller than the former.

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