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First-principles study of magnetic hyperfine field at Cd probe in Co-doped ZnO semiconductor

Diluted magnetic semiconductor systems (DMS) have been widely studied in last years by different experimental techniques as well as by ab-initio calculations in an attempt to clarify the origin of the ferromagnetic order which is observed in several experiments. In general, magnetic order in samples of wide band-gap semiconductor oxides doped with transition metal elements is more likely to occur when they show structural defects, and such magnetism is claimed to be mediated by them. Among these systems, Co-doped ZnO has been intensively investigated and many experiments observed magnetic ordering in samples of this compound whereas many other did not. One experiment, in particular, demonstrated unambiguously a magnetic hyperfine field (mhf) at 111Cd probe nuclei substituting Zn sites in Zn0.9Co0.1O bulk samples [1]. The experiment was performed by means of Perturbed gamma–gamma Angular Correlation spectroscopy (PAC) which is able to observe local fields with an atomic scale. The aim of this work is to search for possible magnetic mechanisms which can originate a magnetic hyperfine field at Cd ion located in Zn site of Co-doped ZnO matrix by means of first-principles calculations. Our ab-initio calculations were developed under Density Functional Theory (DFT) framework using Linearized Augment Plane Waves method (LAPW) embodied within WIEN2k code [2]. The calculations were performed with some different ZnO supercells with diluted Co and/or Cd ions. For the exchange and correlation functionals, both the LDA and GGA approximations were tested. We have verified that calculated mhf and electric field gradient at Cd probe located in cation site of ZnO-Co supercell are in good agreement with the experimental values reported in reference [1]. Furthermore, results at Cd ion neighborhoods show that magnetic moments are transferred from Co ions towards Cd ions, by means of a super-exchange effect, which is mediated by Oxygen ions. References [1] M.E. Mercúrio, A.W. Carbonari et al., J. Magn. Magn. Mater. 322, 1195 (2010). [2] Blaha, P., Schwarz, K., Madsen, G.K.H., Kvasnicka, D., Luitz, J.: WIEN2K, an Augmented Plane Wave plus Local Orbitals Program for Calculating Cristal Properties. Karlheinz Schwarz, Techn. Universität Wien, Austria. ISBN 3-9501031-1-2 (2001).

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