X-ray magnetic dichroism in the (Zn,Co)O diluted magnetic semiconductors from *ab initio* calculations

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Diluted magnetic semiconductors (DMSs), obtained by doping magnetic element as impurity into the host semiconductor, can be used for spintronic devices. As a wide-band-gap II-VI semiconductor, ZnO has recently been considered as a base material for realizing transparent DMSs.

Using the fully relativistic Dirac linear muffin-tin orbital (LMTO) band structure method, we have investigated theoretically from first principles the electronic structure of $(Zn_{1-x}Co_x)O$ DMSs, the x-ray absorption spectra (XAS), x-ray magnetic circular dichroism (XMCD), and x-ray linear dichroism (XLD) spectra at the Co, Zn, and O K and Zn, Co $L_{2,3}$ edges.

Since the local density approximationfails to describe correctly strongly localized d states in ZnO we treated these states within the LSDA+U approach. The effective on-site Coulomb repulsion U wasconsidered as an adjustable parameter. The application of LSDA+U leads to a shift of the Znd statesdownward in energy and makes the bandgap larger (2.12 eV within the LSDA+U versus 0.8 eV within the LSDA in pure ZnOwurtzite). The same effect can be achieved treating the Zn d states as core states. In our calculations we tried both approaches and did not find any significant difference in the XAS and XMCD spectra. The Co d states were treated within the LSDA as well as the LSDA+U approach. We tried various U values for the description of the XAS and XMCD spectra and found that the agreementbetween the theoretically calculated and experimental spectra does not significantly changes in comparison with the LSDA method.

The theory reproduced the shape and energy positions ofmajor fine structures of the Co XAS, XLD, andXMCD spectra at the K and $L_{2,3}$ edges reasonablywell. We found that oxygendeficiencyis responsibleforsome fine structures of the Co L_3 XAS and XMCD spectra and hasminorinfluence on the shape of theO and Zn K x-rayabsorption spectra.

We found that a small peak at about 528 eV at the O K edge XAS evolveswith Co doping, and its intensity increases with Coconcentration suggesting a strong hybridization of O $2p$states with Co $3d$states. This featureoriginates in the Codoped ZnO alloys, and it is ascribed to dipole transitions from O $1s$ to O$2p$ states that are hybridized with the unoccupied $3d$ states ofCo. Thus, the intensityof this peak is a fingerprint of the Co $3d$ density of states.A continuous increase of this peak with Co dopingindicatesmore unoccupied states at the Co $3d$ levels.