X-ray magnetic dichroism in the (Zn,Co)O diluted magnetic semiconductors from first principle calculations.

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Abstract

The electronic structure of the (Zn,Co)O diluted magnetic semiconductors (DMSs) were investigated theoretically from first principles, using the fully relativistic Dirac linear muffin-tin orbital band structure method. The electronic structure was obtained with the local spin-density approximation. 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 were investigated theoretically from first principles. The origin of the XMCD and XLD spectra in these compounds was examined. The orientation dependence of the XAS at the Co and Zn K edges were investigated by calculating the XAS spectra for the $\langle 001 \rangle$ and $\langle 110 \rangle$ magnetization axis. The calculated results are compared with available experimental data.

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