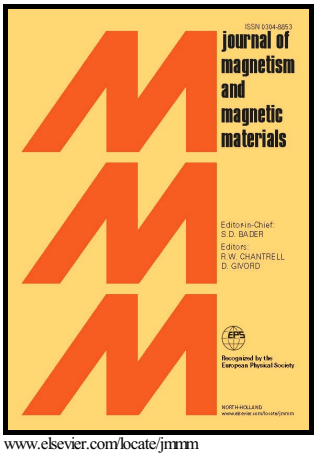

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Magneto-optical Kerr effect in $ZnTMO_2$ (TM= Cr, Mn, Fe, Co and Ni)

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Abstract

First principles generalized gradient full potential density-functional calculations were performed to predict the optical and magneto-optical (MO) properties of the chalcopyrite compounds $ZnTMO_2$, TM= Cr, Mn, Fe, Co and Ni. Detailed investigation of the electronic band structure and density of states is reported. The optical properties in the 0-8 eV energy range are analyzed in terms of band structure transitions. As for the magneto–optical properties, our results show that the studied compounds have peaks in the Kerr rotation ranging from infrared to ultraviolet radiation, with $ZnFeO_2$ having the highest Kerr rotation angle of 10° and -8.46° at 0.35 eV and 4.59 eV, respectively. The peaks in the Kerr spectra were assigned to the optical and magneto–optic contributions. Our calculated function of merit for these compounds indicates that these compounds might be useful for technological application in high density storage.

Key words: : Chalcopyrite; Ab initio calculations; Optical conductivity; Magneto-optical properties; FP-LAPW

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