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R. Merikhi, B. Bennecer, A. Hamidani



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

R. Merikhi, B. Bennecer* and A. Hamidani

Physics Laboratory at Guelma, Faculty of Mathematics, Computing and Material Sciences , University 8 Mai 1945 Guelma, P.O. Box 401 Guelma 24000, Algeria

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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