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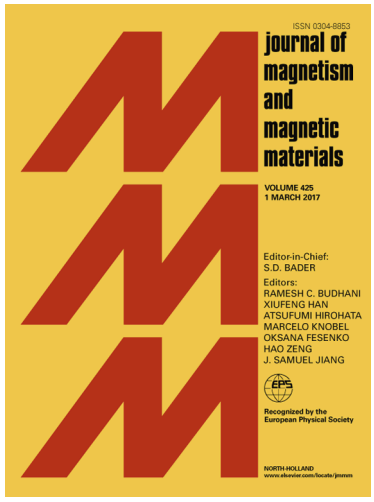

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R. Lamouri, M. Tadout, M. Hamedoun, A. Benyoussef, H. Ez-zahraouy, M. Benaissa, O. Mounkachi

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Effect of the cations distribution on the magnetic properties of $SnFe_2O_4$: First-principles study

R. Lamouri[1,2], M. Tadout[1,2], M. Hamedoun[1], A. Benyoussef[1,2,3], H. Ez-zahraouy[2], M. Benaissa[2], and O. Mounkachi[1,*]

(1) Materials and Nanomaterials Center, MAScIR Foundation , Rabat Design Center Rue Mohamed Al Jazouli – Madinat Al Irfane , Rabat 10 100 – Morocco

(2) LaMCScI (ex LMPHE), B.P. 1014, Faculty of science-Mohammed V University, Rabat, Morocco

(3) Hassan II Academy of Science and Technology, Rabat, Morocco,

Corresponding authors: **o.mounkachi@mascir.com , o.mounkachi@gmail.com**

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Abstract:

In this work, a study of the electronic and magnetic properties of $SnFe_2O_4$ spinel ferrite for different case of octahedral and tetrahedral distribution was carried out by using the Full Potential Linearized Plane Wave (FP-LAPW) method in density functional theory (DFT) implemented in the Wien2k package, with the generalized gradient (GGA) and Tran-Blaha modified Becke-Johnson approximations for the exchange and correlation functional. Our spin-polarized calculations based on mBJ correction show a half metallic behavior for $SnFe_2O_4$ which confirm the usefulness of $SnFe_2O_4$ in spintronic application. From the magnetic properties calculations, it is found that the magnetic moment per formula unit is 8.0327 μ_β, 0.000015 μ_β and 3.99μ_β in $SnFe_2O_4$ 100% normal, 100% inverse and 50 % inverse, respectively .

Keywords: $SnFe_2O_4$, Spinel ferrites, Spintronic, ab initio calculation, FP-LAPW method.

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