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First principles study of magnetic properties of Zn-Sn substituted M-type Sr-hexaferrite SEONG-GON KIM, LAALITHA LIYANAGE, Department of physics and astronomy, Mississippi state university, JEFF HOUZE, None, SUNGHO KIM, Center for advanced vehicular systems, Mississippi state univeristy — Site occupancy and magnetic properties of Zn-Sn substituted M-type Sr-hexaferrite $SrFe_{12-x}(Zn_{0.5}Sn_{0.5})_xO_{19}$ with $x = 1$ were studied using density functional theory and generalized gradient approximation (GGA). Using the GGA+U method the description of strongly correlated $3d$ electrons of Fe was improved. Our results show that Zn and Sn atoms prefer to occupy $4f_1$ and $4f_2$ sites respectively. Favorable Zn-Sn substituted configurations show an increase in saturation of magnetization (M_s), and a decrease in magnetic anisotropy energy (MAE), over the pure M-type Sr-hexaferrite ($x = 0$). Experimental observations agree with the decrease of MAE and the increase of M_s for Zn-Sn substituted Sr-hexaferrite.

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