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First principles study of Al substituted strontium hexaferrite VIVEK DIKSHIT, SULTANA ABABTIN, CHANDANI NANDADASA, SUNGHO KIM, SEONG-GON KIM, Mississippi State University, JIHOON PARK, YANG-KI HONG, The University of Alabama — We have studied the site occupancy and magnetic properties of Al substituted M-type Strontium hexaferrite, $SrFe_{12-x}Al_xO_{19}$ with x = 0.5 and x = 1.0 using density functional theory (DFT). For x = 0.5 case, an Al atom preferentially occupy the 2a site at T = 0 K, this trend endures up to 220 K beyond this temperature Al atom is more likely to occupy the 12k site. For the x = 1.0 case, the site preference probability is maximum when two Al atoms occupy the 2a and the 12k sites. We found that magnetic anisotropy of SrFe12-xAlxO19 increases as the concentration of Al atoms increases, while there is a reduction in the magnetic moment per unit cell by 5μB and 10μB in the case of x = 0.5 and x = 1.0, respectively. Our results agree with the available experimental results on Al substituted strontium hexaferrite.

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