First principles study of magnetism and defect energetics in non-stoichiometric \( \text{Sr}_2\text{FeMoO}_6 \) R. MISHRA, O.D. RESTREPO, W. WINDL, P.M. WOODWARD, The Ohio State University — The influence of disorder and stoichiometry-breaking point defects on the structural and magnetic properties of \( \text{Sr}_2\text{FeMoO}_6 \) have been investigated with the help of electronic structure calculations within the GGA+U approach. Defining the chemical potentials of the constituent elements from constitutional defects, we calculate the energetics of the possible point defects in non-stoichiometric \( \text{Sr}_2\text{FeMoO}_6 \) and find transition metal-ion antisites and oxygen vacancies to be the dominant point defects. In non-stoichiometric \( \text{Sr}_2\text{Fe}_{1+x}\text{Mo}_{1-x}\text{O}_6 \), both \( \text{Fe}_{\text{Mo}} \) antisites and \( \text{Mo}_{\text{Fe}} \) antisites lead to a systematic decrease in saturation magnetization (\( M_s \)). Only \( \text{Mo}_{\text{Fe}} \) antisites destroy the half metallic character of the electronic structure. Oxygen vacancies also reduce the \( M_s \), but the half-metallicity is retained. The optimized unit cell lattice parameters stay within a relatively narrow range despite large changes in composition. In stoichiometric \( \text{Sr}_2\text{FeMoO}_6 \), the \( M_s \) decreases linearly with increasing Fe/Mo antisite disorder with loss in half-metallicity. The calculated results are in excellent quantitative agreement with experimental values.

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