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First principles study of magnetism and defect energetics in non-stoichiometric Sr_2FeMoO_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 Sr_2FeMoO_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 Sr_2FeMoO_6 and find transition metal-ion antisites and oxygen vacancies to be the dominant point defects. In non-stoichiometric $Sr_2Fe_{1+x}Mo_{1-x}O_6$, both Fe_{Mo} antisites and Mo_{Fe} antisites lead to a systematic decrease in saturation magnetization (M_s). Only Mo_{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 Sr_2FeMoO_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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