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Effects of disorder in the Sr_2FeMoO_6 double perovskite via first principles calculations. O. NAVARRO, A.M. REYES, Unidad Morelia, Instituto de Investigaciones en Materiales, Universidad Nacional Autnoma de Mxico, Y. ARREDONDO, Escuela Nacional de Estudios Superiores, Unidad Morelia, Universidad Nacional Autnoma de Mxico — First principles calculations were done in the double perovskite Sr_2FeMoO_6 regarding the effects of cationic disorder and electronic correlation in the ground-state properties such as spin polarization and magnetic moment. We used the Generalized Gradient Approximation (GGA) method including a U Hubbard term. Disorder is introduced via atomic substitution with a ratio of 25% and 12.5%. It is found a magnetic saturation of 2.22_B and 2.99_B for 25% and 12.5% of disorder respectively, in agreement with neutron magnetic scattering experiments. The half-metallic behavior of the above double perovskite remains only for a 12.5% of disorder.

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