MS19-P03 | MAGNETISM IN DOUBLE PEROVSKITES Ba_2CrMoO_6

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Cubic Ba_2CrMoO_6 double perovskite (see Fig.1) is studied using the full potential linearized augmented plane wave (FP-LAPW) method within the frame work of density functional theory (DFT). The structural, electronic and magnetic properties are calculated by using the GGA approximation, GGA+U and MBJ-GGA. Density of states and band structure results reveal a half-metallic ferromagnetic ground state for this component. The mBJ calculations yield a better energy-gap than the GGA and GGA+*U* methods. Our results make the Ba_2CrMoO_6 double perovskite to be a promising candidate for the spintronic application.