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First Principle Calculations of Magnetic and Electronic Properties of Double Perovskite Ba2MnMoO6

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Abstract : The electronic and magnetic structures of double perovskite Ba2MnMoO6 are systematically investigated using the first principle method of the Full Potential Linear Augmented Plane Waves Plus the Local Orbitals (FP-LAPW+LO) within the Local Spin Density Approximation (LSDA) and the Generalized Gradient Approximation (GGA). In order to take into account the strong on-site Coulomb interaction, we included the Hubbard correlation terms: LSDA+U and GGA+U approaches. Whereas half-metallic ferromagnetic character is observed due to dominant Mn spin-up and Mo spin-down contributions insulating ground state is obtained. The LSDA+U and GGA+U calculations yield better agreement with the theoretical and the experimental results than LSDA and GGA do.

Keywords : electronic structure, double perovskite, first principles, Ba2MnMoO6, half-metallic
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