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First Principle Studies on the Structural, Electronic and Magnetic Properties of Some BaMn-Based Double Perovskites

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Abstract : Perovskite materials which include magnetic elements have relevance due to the technological perspectives in the spintronics industry. In this work, we have investigated the structural, electronic and magnetic properties of double perovskites Ba2MnXO6 with X= Mo and W by using the full-potential linearized augmented plane wave (FP-LAPW) method based on Density Functional Theory (DFT) [1, 2] as implemented in the WIEN2K [3] code. The interchange-correlation potential was included through the generalized gradient approximation (GGA) [4] as well as taking into account the on-site coulomb repulsive interaction in (GGA+U) approach. We have analyzed the structural parameters, charge and spin densities, total and partial densities of states. The results show that the materials crystallize in the 225 space group (Fm-3m) and have a lattice parameter of about 7.97 Å and 7.95 Å for Ba2MnMoO6 and Ba2MnWO6, respectively. The band structures reveal a metallic ferromagnetic (FM) ground state in Ba2MnMoO6 and half-metallic (HM) ferromagnetic (FM) ground state in the Ba2MnWO6 compound, with total magnetic moment equal 2.9951μB (Ba2MnMoO6) and 4.0001μB (Ba2MnWO6). The GGA+U calculations predict an energy gap in the spin-up bands in Ba2MnWO6. So we estimate that this material with HM-FM nature implies a promising application in spin-electronics technology.

Keywords : double perovskites, electronic structure, first-principles, semiconductors
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