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Density functional investigation of the spin frustration and the field-driven long-range ordering in the honeycomb lattice system $Bi_3Mn_4O_{12}(NO_3)$ JIA LIU, WON-JOON SON, MIKE WHANGBO, NCSU — $Bi_3Mn_4O_{12}(NO_3)$, consisting of the honeycomb lattices of Mn^{4+} (d^3) ions, has dominant antiferromagnetic interactions ($\theta_{CW} = -257$ K) but its spins do not order down to 0.4 K. However, applied magnetic fields induce a long-range magnetic order, which is believed to arise from the spin canting due to the Dzyaloshinskii-Moriya interaction. To explain these observations, we examined the spin exchanges between the Mn^{4+} ions (J_1, J_2, J_c) by DFT+U calculations and the preferred orientation of their spins by DFT+U+SOC calculations. The spin frustration is reproduced by U close to zero with $J_2/J_1 \approx 1/2$. The cause for the field-induced long-range magnetic ordering was explored on the basis of DFT+U+SOC calculations.

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