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Atomic and magnetic structures of (CuCl)$LaNb_2O_7$ and (CuBr)$LaNb_2O_7$: Density functional calculations CHUNG-YUAN REN, Department of Physics, National Kaohsiung Normal University,Taiwan, CHING CHENG — The atomic and magnetic structures of (CuX)$LaNb_2O_7$ (X=Cl and Br) are investigated using the density-functional calculations. Among several tens of the examined structures, an orthorhombic distorted 2×2 structure, in which the displacement pattern of X halogens resembles the model conjectured previously based on the empirical information is identified as the most stable one. The displacements of X halogens, together with those of Cu ions, result in the formation of X-Cu-X-Cu-X zigzag chains in the two materials. The nearest-neighbor interaction within the zigzag chains are determined to be antiferromagnetic (AFM) for (CuCl)$LaNb_2O_7$ but ferromagnetic (FM) for (CuBr)$LaNb_2O_7$. On the other hand, the first two neighboring interactions between the Cu cations from adjacent chains are found to be AFM and FM respectively for both compounds. The magnitudes of all these in-plane exchange couplings in (CuBr)$LaNb_2O_7$ are evaluated to be about three times those in (CuCl)$LaNb_2O_7$. In addition, a sizable AFM inter-plane interaction is discovered between the Cu ions separated by two NbO_6 octahedra. The present study strongly suggests the necessity to go beyond the square $J_1 - J_2$ model in order to correctly interpret the magnetic property of (CuX)$LaNb_2O_7$.

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