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Single-ion Anisotropy, Dzyaloshinskii-Moriya Interaction and Negative Magnetoresistance of the Spin-1/2 Pyrochlores R2V2O7
HONGJUN XIANG, Fudan University, ERJUN KAN, M.-H. WHANGBO, C. LEE, North Carolina State University, SU-HUAI WEI, National Renewable Energy Laboratory, X.G. GONG, Fudan University — The electronic and magnetic properties of spin-1/2 pyrochlores $R_2V_2O_7$ were investigated on the basis of density-functional calculations. Contrary to the common belief, the spin-1/2 V^{4+} ions are found to have a substantial easy-axis single-ion anisotropy. The $|D/J|$ ratio deduced from the magnon quantum Hall effect of $Lu_2V_2O_7$, where J is the nearest-neighbor spin exchange and D is the Dzyaloshinskii-Moriya parameter, is much greater than the value estimated from our calculations (i.e., 0.32 vs. 0.05). We show that this discrepancy is due to the neglect of the single-ion anisotropy of the V^{4+} ions, and the negative magnetoresistance observed for $R_2V_2O_7$ arises from a new mechanism.

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