

Abstract Submitted
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New **natural**
spin-1/2 kagomé systems — kapellasite $\text{Cu}_3\text{Zn}(\text{OH})_6\text{Cl}_2$ and haydeeite $\text{Cu}_3\text{Mg}(\text{OH})_6\text{Cl}_2$ OLEG JANSON, HELGE ROSNER, Max-Planck-Institute for Chemical Physics of Solids Dresden, Germany — New natural spin-1/2 systems with kagomé layers — kapellasite $\text{Cu}_3\text{Zn}(\text{OH})_6\text{Cl}_2$ and haydeeite $\text{Cu}_3\text{Mg}(\text{OH})_6\text{Cl}_2$ — are studied by full potential density functional calculations using the fplo6.00-24 code. The band structure, obtained by a paramagnetic calculation, was used to solve a tight-binding model. The transfer integrals were mapped subsequently to a Hubbard model and to a Heisenberg model, giving an estimate for the antiferromagnetic (AF) exchange. The total exchange, containing AF and ferromagnetic (FM) parts, was derived from LSDA + U supercell calculations. As the main result, we find that in both compounds only two exchange integrals are relevant: the nearest neighbour exchange J_1 and the interaction J_d along the diagonals of the Cu^{2+} hexagons. Surprisingly, the size of these integrals depends strongly on the O—H bond length which was therefor optimized with respect to the total energy, resulting in about 1 Å for both compounds. Using the optimized O—H bond length, we find $J_1 > J_d$ in kapellasite and $J_1 \sim J_d$ in haydeeite. According to our results, kapellasite can be described as a modified kagomé lattice, while interpenetrating chains should be considered for haydeeite. Our results should encourage new experimental studies of these interesting materials.

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