Abstract Submitted
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Study of the magnetic structures of the atacamite and botallackite forms of $Cu_2(OH)_3Cl$ in terms of first principles DFT calculations[1] JINHEE KANG, CHANGHOON LEE, MIKE H. WHANGBO, Department of Chemistry, North Carolina State University — The atacamite and botallackite forms of $Cu_2Cl(OH)_3$ are made up of edge- and corner-sharing $Cu(OH)_4Cl_2$ octahedra. Each polymorph consists of two slightly different types of $Cu(OH)_4Cl_2$ octahedra, with their Cu x^2-y^2 magnetic orbitals contained in the $Cu(OH)_4$ square planes. Atacamite and botallackite are different in the way the $Cu(OH)_4$ square planes are connected, but their magnetic properties of atacamite and botallackite are quite similar. To explain these observations, the crystal structures of the two polymorphs were optimized by first principles DFT calculations. We then evaluated the spin exchange interactions of the two polymorphs using the optimized structures on the basis of DFT calculations. To a first approximation, both polymorphs were found to be described by a uniform 1D antiferromagetic chain model with spin frustration arising from the next-nearest-neighbor interactions. Implications of these observations were explored.

[1]DMSE, OBES, and DOE

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