Naturally frustrated: a computational study of spin-1/2 kagome minerals

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In recent years, considerable efforts were spent to search for materials with a kagome arrangement of spin-1/2 ions. Such systems are expected to imply exotic magnetic properties arising from the magnetic frustration and the magnetic ground state where constituent spins do not freeze (the spin liquid). Still, real material realizations of a spin-1/2 kagome lattice are scarce. Quite unexpectedly, the majority of the candidate systems are natural minerals: herbertsmithite $Cu_3Zn(OH)_6Cl_2$, its polymorph kapellasite $Cu_3Zn(OH)_6Cl_2$, haydeeite $Cu_3Mg(OH)_6Cl_2$ and volborthite $Cu_3[V_2O_7](OH)_2{\cdot}2H_2O$.

However, subsequent studies revealed that the simple kagome model fails to describe the magnetism of these minerals. Moreover, the compounds appeared to be rather different with respect to their experimental behaviour. To account for the disagreement between model theory and experiment, we preformed a systematic microscopic analysis using full potential density functional theory (DFT) calculations, that can provide the relevant orbitals and model parameters. Subsequently, we simulate the ground state properties and lowest lying magnetic excitations by exact diagonalization studies.

In the isostructural systems kapellasite and haydeeite, the non-magnetic cations occupy the cavities of a kagome network and, as revealed by our analysis, have a considerable influence on the magnetic properties [1]. Quite unexpectedly, we nd an additional relevant magnetic coupling, which modifies the ground state and the excitation spectrum. The availability of the two isostructural compounds allows for a systematic study of the influence of a non-magnetic cation. Surprisingly, we found a large influence of the side group (OH) on the leading magnetic exchanges which underlines the crucial importance of an accurate structural input.

Experimental data on volborthite were generally considered within the anisotropic kagome model arising from a seemingly small monoclinic distortion of the kagome network. However, DFT calculations and numerical simulations yield an essentially different magnetic model of coupled quantum spin 1/2 chains with ferromagnetic first and antiferromagnetic second neighbour coupling [2]. As an essential feature of the magnetic model, our DFT calculations reveal the orbital order rarely observed in cuprates. Exact diagonalization studies reveal improved agreement with experiments. In conclusion, the applied microscopic approach is an appropriate tool to extend our understanding about the “structure-property” relation of correlated magnetic insulators.

References

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