

「フロンティア機能性物質創製センター」 オープンセミナーのご案内

連絡先 坂井徹 (物質理学研究科)

TEL: 0791-58-0151 E-mail: sakai@sci.u-hyogo.ac.jp

「フロンティア機能性物質創製センター」では、オープンセミナーを開催しております。第29回は、岡山大学異分野基礎科学研究所・Jeschke 教授にご講演をお願いしました。多くの方々のご来聴をお待ちしています。

兵庫県立大学「フロンティア機能性物質創製センター」
オープンセミナー(第29回)

講師 : Harald O. Jeschke 教授
(岡山大学異分野基礎科学研究所)

“Search for spin liquids in kagome and pyrochlore materials”

Herbertsmithite $\text{ZnCu}_3(\text{OH})_6\text{Cl}_2$ is one of the best candidates for a quantum spin liquid; its Cu^{2+} ions form a kagome lattice. With half-filled Cu $d_{x^2-y^2}$ bands, it is a Mott insulator. We have determined the parameters of the underlying Heisenberg Hamiltonian using density functional theory (DFT) methods. The tendency of herbertsmithite to some Cu/Zn disorder has led to the investigation of closely related kagome materials with different arrangement of kagome planes. Barlowite $\text{Cu}_4(\text{OH})_6\text{FBr}$ is a canted antiferromagnet. We have proposed to replace the interstitial Cu by a nonmagnetic metal ion in order to obtain another highly frustrated kagome material. Our prediction that such a material should be a very good spin liquid candidate has recently been confirmed experimentally.

An interesting polymorph of herbertsmithite is kapellasite which orders magnetically and has a ferromagnetic nearest neighbour exchange coupling. We discuss the positioning of kapellasite $\text{ZnCu}_3(\text{OH})_6\text{Cl}_2$, haydeeite $\text{MgCu}_3(\text{OH})_6\text{Cl}_2$ and hypothetical $\text{CdCu}_3(\text{OH})_6\text{Cl}_2$ in the phase diagram of the J_1 - J_2 - J_3 Heisenberg model. We find kapellasite and haydeeite to be near the boundaries between magnetically ordered and disordered phases, and we predict that moderate pressures could bring the materials into the paramagnetic regime.

We also investigate the low-temperature phase of the recently synthesized $\text{Lu}_2\text{Mo}_2\text{O}_5\text{N}_2$ material, a rare realization of an $S = 1/2$ three-dimensional pyrochlore Heisenberg antiferromagnet in which Mo^{5+} are the $S = 1/2$ magnetic species. Using density functional theory, we find that the compound is well described by a Heisenberg model with exchange parameters up to third nearest neighbors. The analysis of this model via the pseudofermion functional renormalization group method reveals paramagnetic behavior down to a temperature of at least $T = |\theta_{\text{CW}}|/100$, in agreement with the experimental findings hinting at a possible three-dimensional quantum spin liquid.

日時 : 2018 年 4 月 10 日 (火曜日)

14:00 ~ 15:00

場所 : SPring-8 「萌光館」