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Surprises in low dimensional spin 1/2 magnets - from crystal chemistry to microscopic magnetic models of complex oxides

HELGE ROSNER, MPI CPfS Dresden

A microscopic understanding of the structure-properties relation in crystalline materials is a main goal of modern solid state chemistry and physics. Due to their peculiar magnetism, low dimensional spin 1/2 systems are often highly sensitive to structural details. Seemingly unimportant structural details can be crucial for the magnetic ground state of a compound, especially in the case of competing interactions, frustration and near-degeneracy. Here, we present for selected, complex Cu^{2+} systems that a first principles based approach can reliably provide the correct magnetic model, especially in cases where the interpretation of experimental data meets serious difficulties or fails. We demonstrate that the magnetism of low dimensional insulators crucially depends on the magnetically active orbitals which are determined by details of the ligand field of the magnetic cation. Our theoretical results are in very good agreement with thermodynamic and spectroscopic data and provide deep microscopic insight into topical low dimensional magnets.