**MS26 Quantum mechanical models for dynamics and diffuse scattering**

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Pauflerite β-$VOSO_4$ as a 1D S = 1/2 Heisenberg antiferromagnetic system: crystal structure, disorder, and thermal expansivity

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Abstract

Low-dimensional antiferromagnets are of interest both from a fundamental point of view, and as perspective materials for future spintronics applications. Similar to some vanadyl phosphates, Pauflerite β-$VOSO_4$ is a quasi–one-dimensional S = 1/2 Heisenberg system[1]. We report on the low-temperature thermal expansion of a synthetic β-$VOSO_4$, revealing a structural rationale for the magnetic chain direction in agreement with inelastic neutron scattering measurements and DFT calculations, as well as the observation of diffuse scattering. We provide a microscopic interpretation of the underlying correlated disorder, which is linked to the inversion of the short-long V-O distance pairs along the chains, forming a local defect state. Diffuse scattering indicates that such defects are correlated and form thin layers, destroying alternation of V-O bonding pattern in the neighbouring chains. Using direct Monte Carlo (MC) modelling[2], we present here an atomistic realization of the disordered crystal structure. 2D defects in anisotropic magnetic systems may perturb, or even destroy, long-range magnetic ordering. In particular, the lack of inversion symmetry in the 2D defect layers opens the possibility for the Dzyaloshinskii-Moriya interaction (DMI) and, consequently, chiral magnetism localized in the defect planes. In this respect, the defect β-$VOSO_4$ structure offers a new, and as yet unexplored, playground.

References

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