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Modelling diffuse magnetic scattering in a "partial spin-liquid" kagomé compound

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Fe4Si2Sn7O16 has a well-ordered complex composite layered structure that incorporates perfectly hexagonal kagomé lattices of high-spin Fe2+ (S = 2) cations. Below TN = 3.5 K it adopts a unique "striped" magnetic structure [1,2] that breaks hexagonal symmetry and leaves 1/3 of the spins geometrically frustrated in an apparent "partial spin-liquid" state down to at least 40 mK. Polarised neutron diffraction data collected on D7 at the ILL show persistent structured magnetic diffuse scattering below TN, consistent with short-range interactions among 1/3 of the HS Fe2+ sites. We have fit the diffuse magnetic scattering intensity with a Monte Carlo "big box" approach and a magnetic interaction approach. The determined signs and relative magnitudes of the spin exchange coupling are consistent between these two approaches and with the results of high-level DFT (meta-GGA SCAN functional) calculations. Our key result is that the first, second and third-nearest neighbour exchange interactions (J1, J2, J3) are all strongly antiferromagnetic. This may explain why Fe4Si2Sn7O16 does not adopt either of the conventional long-range-ordered kagomé states that preserve hexagonal symmetry: q = 0 "in-out", in which third-nearest neighbours are ferromagnetic with respect to each other; or q = $\sqrt{3}\times\sqrt{3}$ "spiral", in which second-nearest neighbours are ferromagnetic with respect to each other. We propose that the partially ordered ground state of Fe4Si2Sn7O16, in which there are no strictly ferromagnetic relationships, is the best compromise when J1-3 are all strongly antiferromagnetic.

[1] CD Ling et al., Physical Review B 9 (2017) 180410
[2] S Dengre et al., Physical Review B 103 (2021) 064425

Topics

Magnetism and Condensed Matter

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