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The Magnetic Exchange Pathways of Fe4Si2Sn7O16

Below TN = 3.0 K, the bi-layered Fe4Si2Sn7O16 possesses a frustrated Kagome lattice of Fe sites within its FeO6/SnO6 oxide layer1. This magnetic structure contains canted AFM chains whose sites are AFM w.r.t. neighbouring chain sites along y and xy (bridged by NM Sn and frustrated Fe sites) and along z (~9 Å apart and through a non-magnetic FeSn6 cluster layer).

DFT calculations of the electronic and magnetic structure of Fe4Si2Sn7O16 are used to investigate the mechanisms behind the intralayer and interlayer magnetic ordering. Initial bonding analysis of the oxide layer show possible separate AFM super-exchange pathways along x and y, with an additional pathway proposed in 20171 also being investigated alongside (an AFM 'super-super' exchange between diagonally opposite sites along xy and y).

The question of the exact state bonding and charge distribution within the cluster layer has also been investigated computationally as this would be a critical factor affecting the interlayer ordering.

Similar structural trends were seen in computational models with Ru substitution into the cluster layer and with Mn doping into the oxide layer, the latter is in line with NPD studies of Fe1.45Mn2Si2.55Sn7O16 which shows the same magnetic ordering as Fe4Si2Sn7O162. Future NPD studies of Ru and simultaneous Ru/Mn substituted compounds are being pursued to compliment this theoretical work.

Topic

Physics

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