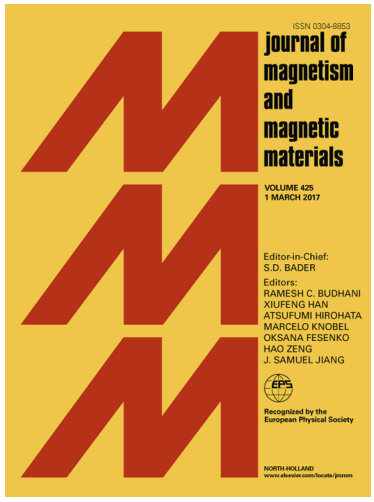

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A comprehensive study of magnetic exchanges in the layered oxychalcogenides $Sr_3Fe_2O_5Cu_2Q_2$ (Q= S, Se)

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Abstract

The layered oxysulfide $Sr_3Fe_2O_5Cu_2S_2$ was prepared, and its crystal structure and magnetic properties were characterized by synchrotron x-ray diffraction (XRD), powder neutron diffraction (PND), Mössbauer spectroscopy measurements and by density functional theory (DFT) calculations. In addition, the spin exchange interactions leading to the ordered magnetic structure of $Sr_3Fe_2O_5Cu_2S_2$ were compared with those of its selenium analogue $Sr_3Fe_2O_5Cu_2Se_2$. The oxysulfide $Sr_3Fe_2O_5Cu_2S_2$ adopts a G-type antiferromagnetic (AFM) structure at a