Site Mixing and complex magnetic structures in topological insulators MnBi2Te4 and MnSb2Te4

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Intrinsic magnetic topological insulators (TIs) provide a fertile playground to study exotic quantum states related to nontrivial band topologies, including the quantum anomalous Hall insulators and axion insulators. With the recent report of MnBi2Te4 as the first instance of an intrinsic antiferromagnetic TI, MnX2Te4 (X= Bi, Sb) and their family members have captured much interest. MnX2Te4 are van der Waals (vdW) quantum magnets, and each 2D layer consists of septuple atomic layers that are weakly bound to each other by vdW forces. However, real crystals have structural imperfections, and the MnX2Te4 family members show significant Mn/Bi(Sb) site mixing. Here we present single-crystal neutron studies on the chemical and magnetic structures of MnBi2Te4 and MnSb2Te4. We have found that the Mn ions on both Mn and Bi (Sb) sites form a long-range magnetic order at low temperatures, forming ferrimagnetic septuple layers. Therefore, the magnetic ground states of MnX2Te4 are more than a simple A-type antiferromagnetic ground state, as usually assumed.

The site mixing levels depend on the detailed sample growth conditions, and MnSb2Te4 shows a higher site mixing level than MnBi2Te4. We have found that for MnSb2Te4, the magnetic interaction between the neighboring septuple layers shows an interesting correlation with the Mn/Sb site mixing levels, which can be either antiferromagnetic or ferromagnetic [1]. This finding suggests site-mixing as a knob to engineering the magnetic ground states for these intriguing topological materials.

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[1] Liu, Yaohua et al., "Site mixing for engineering magnetic topological insulators." Physical Review X 11, 021033 (2021)