Study of the honeycomb lattice material $(Mn_{0.5}Ni_{0.5})_2Mo_3O_8$

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The compound $(TM)_2Mo_3O_8$ (TM = transition metal) has emerged as a widely studied platform for exploring exotic phenomena in condensed matter physics, owing to its honeycomb lattice structure and the rich variety of magnetic and thermodynamic behaviors it hosts. Parent compounds such as $Mn_2Mo_3O_8$ and $Ni_2Mo_3O_8$ display contrasting properties, including multiferroicity, unconventional spin orientations, and phase transitions below room temperature. Moreover, numerous studies have demonstrated that chemical doping—for example, in $FeNiMo_3O_8$, $MgNiMo_3O_8$, and $FeCoMo_3O_8$—can significantly modify heat capacity, raise transition temperatures, and induce striking anomalies in temperature-dependent electron spin resonance, effects strongly linked to the occupancy of transition metals at tetrahedral and octahedral lattice sites.

Motivated by these insights, we synthesized high-quality $(Mn_{0.5}Ni_{0.5})_2Mo_3O_8$ single crystals using a chemical vapor transport method with iodine and tellurium tetrachloride as transport agents. The structural integrity and purity of the crystals were confirmed by x-ray diffraction, while neutron powder diffraction and magnetization measurements revealed a transition into a ferromagnetic phase below approximately 30 K. Furthermore, detailed analysis of the transition-metal site occupancies and simulations of the magnetic structure provide new evidence for the pivotal role of local lattice environments in governing the emergent magnetic behavior of this class of honeycomb-lattice materials.

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