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Effects of Disorder on Magnetism and Electronic Structure in Kagome Alloy Fe_2MnSn

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Abstract: Iron-based magnets with the Kagome lattice are a rich set of materials due to their non-trivial topology combined with high magnetic ordering temperature (T_c). Previously, we identified and synthesized Fe_2MnSn as a promising material with high magnetic anisotropy characterized by a high T_c. The desirable magnetic properties of ternary alloys are controlled by atomic-level antisite disorder and are sensitive to stoichiometry as well. To illustrate the role of disorder in Fe_2MnSn, we performed DFT calculations using 64-atom supercells, which enabled us to probe changes in the density of states and magnetic moments by design. Our data show that substitution of Mn for Sn modifies the system and reduces the total magnetization, consistent with experiments. Specifically, substitution studies find the total magnetic moment decreases from 7.15 μB/f.u. for Fe_2MnSn to 6.24 μB/f.u. for $Fe_2Mn_{1.25}Sn_{0.75}$. Unlike Mn, which prefers only anti-parallel alignment at Sn sites with respect to the Kagome lattice, Fe stabilizes in both parallel and anti-parallel configurations. We present the effect of such disorder on the density of states and related physical properties, providing new insight into how Kagome alloys can be tuned for spintronic functionality.

Biography: Thayne Dean is a second-year master's student in physics at SIU. He also received his B.S. in physics from SIU in 2025. At SIU, Thayne is in Dr. Dipanjan Mazumdar's lab, computationally studying previously and currently experimentally studied materials in the group. Outside of the lab, you may find Thayne enjoying nature, whether that's hiking, bird watching, or spending time with his partner and their dog.