

Abstract Submitted
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First principles study of lattice disordering and magnetic behavior in CuNiMnAl and CuNiMnSn Heusler alloys SHIFRAH ARON-DINE, Harvey Mudd College, GREGORY POMREHN, The Boeing Company, AURORA PRIBRAM-JONES, Lawrence Livermore National Lab, LORI BASSMAN, Harvey Mudd College — In this work we present density functional theory calculations on two new Heusler alloys, CuNiMnAl and CuNiMnSn, and explore how the electronic properties of these structures are affected by atomic disordering. Elements are disordered 1%-25% on constant and varying sublattices to explore changes in electronic structure and magnetization. We then use a Monte Carlo method to predict expected magnetic behavior and compare with experimental results.

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