Abstract Submitted
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Ab-Initio Insights into Novel Magnetic Behavior in the $Mn_{1-x}Fe_xRu_2Sn$ Pseudo-Binary Heusler[1] ELIZABETH DECOLVENAERE, MICHAEL GORDON, RAM SESHADRI, ANTON VAN DER VEN, Univ of California - Santa Barbara — Many Heusler compounds possess magnetic properties well-suited for applications as spintronic materials. The pseudo-binary $Mn_{0.}5Fe_{0.5}Ru_2Sn$, formed as a solid solution of two full Heuslers, has been recently shown to exhibit exchange-hardening suggestive of two *magnetic* phases, despite only one observed *chemical* phase[1]. We have performed ab-initio studies of over one hundred chemical and magnetic orderings of the $Mn_{1-x}Fe_xRu_2Sn$ pseudo-binary to better understand the unique magnetic behavior developing in this system. Utilizing a mixed-basis chemical-and-magnetic cluster expansion, we find a transition from ferromagnetic (FM) to antiferromagnetic (AFM) behavior dependent on composition, with (111) AFM ordering on the Mn species at equiatomic composition, in agreement with the experimental study. By exploring and examining the ensemble-averaged magnetic and chemical configurations at multiple compositions and temperatures, we identify the mechanism behind the apparent magnetic hardening, driven by alternating planes of FM and AFM-ordered spins at equiatomic and iron-rich compositions. [1] J. Douglas, E. Levin, T. Pollock. J. Castillo, P. Adler, C. Felser, S. Krämer, K. L. Page, R. Seshadri. Phys. Rev. B 94, 094412 (2016)

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