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Dynamic Correlations and the Ground State of MnSi ROBERT D. COLLYER, DANA A. BROWNE, Louisiana State University — MnSi is a metallic helimagnet below 29 K. Above 1.46 GPa, the moment is completely suppressed resulting in an unusual magnetic state. Density functional theory (DFT) predicts that MnSi has a moment of $1.0 \mu_B/Mn$, which is much larger than the measured value of ~0.4 $4\mu_B/Mn$. Additionally, DFT predicts a smaller magnetovolume coupling than found in experiment. We found that the addition of a Hubbard-U reproduces the experimental moment, but worsens the pressure dependence. We explored the effect of dynamic correlations on the pressure dependence of the moment using a fluctuating exchange approximation (FLEX), and contrast our results for MnSi with the B20 form of FeGe, which exhibits similar behaviors.

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