A DFT OF MAGNETIC TENDENCIES IN TiAu

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TiAu is a rare example of a weak antiferromagnetic, ordering below 36 K. Our interest in this intermetallic compound was piqued by the existence of van Hove singularities (vHs) within 4meV of the Fermi level, reminiscent of the weak ferromagnets $ZrZn_2$ and $TiBe_2$. This fine structure leads to a peak in the density of states and to peculiar behavior in the susceptibility, thus may play a role in creating magnetic fluctuations. The vHs is located, with its quadratic energy dispersion corresponding to effective masses (two positive, one negative) differing in magnitude by a factor of five. Morosan's group (private communication) has found that hole doping, viz. $Ti_{1-x}Sc_xAu$, causes the magnetic moment to disappear at x_{cr}=0.13. We apply fixed spin moment calculations and the virtual crystal approximation within DFT to access the tendencies toward ferromagnetism, and among other results find FM instability as well within both LDA and GGA. Several results will be presented and assessed in light of the existing experimental data.

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