

Abstract Submitted
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Theory of electronic and magnetic properties of weak antiferromagnetic TiAu¹ WEN FONG GOH, WARREN PICKETT, Univ of California - Davis — To date, only a few itinerant magnetic compounds have been found, viz. ZrZn₂, TiBe₂ and Sr₃In, all comprised of nonmagnetic elements. TiAu, a newly synthesized itinerant weak antiferromagnet, orders antiferromagnetically below 36 K. Neutron diffraction reveals an ordered local moment of only 0.15 μ_B /Ti at a wave vector $Q=(0,\pi/b,0)$. Hole doping, viz. Ti_{1-x}Sc_xAu, causes the magnetic moment to disappear at a quantum critical point $x_{Sc}=0.13$. We present results of an extensive study of the electronic and magnetic properties of TiAu. DFT calculations reveal van Hove singularities at $(0,0.45\pi/b,0.49\pi/c)$, 4 meV above the Fermi level. Several types of analysis will be discussed: fixed spin moment studies and Stoner enhancement; magnetic energies; magnetism versus doping; Fermi surface nesting; corrections for spin fluctuations.

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