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Density functional determination of the magnetic state of β -MnAs LEONARD KLEINMAN, MANISH NIRANJAN, B.R. SAHU, The University of Texas at Austin — Ferromagnetic hexagonal α -MnAs has a first order phase transition to β -MnAs at about 40 ° C. Because it shows no long range antiferromagnetic order, most workers assume that it is paramagnetic in spite of the fact that it does not have a Curie-Weiss magnetic susceptibility. With the aid of density functional calculations, we show that it is antiferromagnetic and explain the lack of observed long range order.

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