

Abstract Submitted
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Theory of the Magnetic Moment in Iron Pnictides¹ JIANSHENG WU, PHILIP PHILLIPS, Department of Physics, University of Illinois at Urbana-Champaign, ANTONIO CASTRO-NETO, Department of Physics, Boston University — We show that the combined effects of spin-orbit, monoclinic distortion, and p-d hybridization in tetrahedrally coordinated Fe in LaFeAsO invalidates the naive Hund's rule filling of the Fe d-levels. The two highest occupied levels have one electron each but as a result of differing p-d hybridizations, the upper level is more itinerant while electrons in the lower level are more localized. The resulting magnetic moment is highly anisotropic with an in-plane value of $0.25 - 0.35\mu_B$ per Fe and a z-projection of $0.06\mu_B$, both of which are in agreement with experiment.

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