

Abstract Submitted
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Magnetic and orbital ordering in models for pnictides¹ MARIA DAGHOFER, IFW Dresden, Germany, ANDREW NICHOLSON, ADRIANA MOREO, ELBIO DAGOTTO, University of Tennessee and Oak Ridge National Laboratory, TN — While the shape of the Fermi surface (FS) obtained with the local density approximation (LDA) can be reproduced with two orbitals, three orbitals are needed to produce the degeneracy of the hole pockets. We discuss a three-orbital model including the xz , yz , and xy iron orbitals, which qualitatively reproduces the shape and orbital composition of the FS obtained for undoped pnictides by LDA. Since this model is not at half filling, orbital order becomes a possibility in addition to various magnetic phases. We use a mean-field approach and the Variational Cluster Approach to investigate orbital and magnetic order depending on the interaction parameters U and J . With increasing Coulomb repulsion U , four different regimes arise: (1) paramagnetic metal, (2) magnetic metal with $(\pi, 0)$ spin order, (3) metal with $(\pi, 0)$ spin order as well as alternating orbital order, and (4) magnetic and ferro-orbital ordered insulator. We discuss the spectral density and the FS and compare our findings to mean-field results for models with all five iron- d orbitals. M. Daghofer, A. Nicholson, A. Moreo, and E. Dagotto, arXiv:0910.1573

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