Abstract Submitted
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How close is LaOFeAs to Mott transition? A model Hamiltonian calculation within the Gutzwiller approximation[1] YONGXIN YAO, Membership Pending, JÖRG SCHMALIAN, RAFAEL FERNANDES, CAI-ZHUANG WANG, KAI-MING HO, Iowa State University — Using a five-band tight binding model for LaOFeAs we study the role of electron correlations on the low energy electronic structure. The phase boundaries between a metallic state and Mott insulating phases are determined as a function of Coulomb repulsion U and Hund's coupling J for a total number of six d-electrons. For realistic values of U and J LaOFeAs is found to be on the metallic side of the phase boundary. In addition we give a number of spectroscopic signatures that can be used to determine whether the electronic excitations of the metallic state are affected by the vicinity to a Mott transition. These results elucidate the role of strong electron correlations in FeAs-based systems.

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