

Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Effect of Orbital Differentiation on Magnetism in the 111 iron-based superconductors MING-CUI DING, YU-ZHONG ZHANG, Shanghai Key Laboratory of Special Artificial Microstructure Materials and Technology, School of Physics Science and Engineering, Tongji University — Though similar lattice and electronic structures were found in MgFeGe, LiFeAs and NaFeAs, distinct behaviors at low temperature were reported from experiments. While MgFeGe is nonmagnetic and non-superconducting down to 2 K, LiFeAs is a good superconductor with $T_c = 18$ K, which are in sharp contrast to NaFeAs where a magnetically driven structural phase transition above the superconducting transition is detected. By calculating orbitally resolved Pauli susceptibility, we conclude that the occurrence of magnetism and superconductivity in these materials can be well interpreted from the weak coupling limit provided orbital degrees of freedom are considered. The stronger magnetic instability appearing in the $d_{x^2-y^2}$ orbital is responsible for the occurrence of weak magnetism in NaFeAs, compared to the superconducting LiFeAs, while featureless q dependent magnetic instability is responsible for the nonmagnetism in MgFeGe.

Ming-Cui Ding
Shanghai Key Laboratory of Special Artificial Microstructure Materials
and Technology, School of Physics Science and Engineering,
Tongji University

Date submitted: 07 Nov 2013

Electronic form version 1.4