Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Orbital selective Mott physics in the 111 iron pnictides RONG YU, Department of Physics, Renmin University of China, Beijing 100872, China, JIANXIN ZHU, Theoretical Division and Center for Integrated Nanotechnologies, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA, QIMIAO SI, Department of Physics and Astronomy, Rice University, Houston, Texas 77005, USA — Motivated by recent ARPES measurements on the iron pnictides compounds AFeAs (A=Li,Na), we study the effects of electron correlations on the bandstructures in these compounds via microscopic multiorbital Hubbard models using the U(1) slave-spin theory. We find that the calculated phase diagrams of both compounds at the commensurate filling $n = 6$ contain a common orbital selective Mott phase (OSMP) besides a metallic one and a Mott insulating one. The OSMP is stabilized in a much wider parameter range in LiFeAs than in NaFeAs, as a consequence of a larger energy splitting between the Fe d_{xy} orbital and the $d_{xz/yz}$ orbitals, as well as suppressed hoppings between the d_{xy} and $d_{xz/yz}$ orbitals in LiFeAs. Meanwhile, the onset Coulomb coupling for the orbital selective Mott transition (OSMT) in LiFeAs shows a strong temperature dependence. This pushes the LiFeAs system close to an OSMT with a strongly suppressed quasiparticle spectral weight in the d_{xy} orbital at high temperatures, similar to the iron chalcogenides. Our finding indicates that the orbital selective Mott physics is a common feature for both iron pnictides and iron chalcogenides.

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Date submitted: 11 Nov 2016 Electronic form version 1.4