Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

First-principles study of orbital-selective magnetism in FeAs-based superconductors HYUNGJU OH, DONGHAN SHIN, HYOUNG JOON CHOI, Department of Physics and IPAP, Yonsei University — $LaFeAsO_{1-x}F_x$ and related compounds show unconventional superconductivity (SC) in the vicinity of the antiferromagnetism (AFM). These compounds are featured with multiple Fermi surfaces with strong orbital characters. We perform first-principles calculations of the electronic and magnetic properties in LnFeAsO (Ln=La, Ce, Pr, Nd, Sm, and Gd) as a function of Fe magnetic moment to study material-dependent interplay between orbitals and magnetic moments. With this approach, we show orbital-selective magnetic phases in small-Fe-moment regime: d_{xy} magnetic phase, which is itinerantly driven by orbital selection of Fermi-surface nesting, and d_{yz} magnetic phase, which is driven by local interactions. The Fe magnetic moments in the two phases show different coupling strengths to Fermi-surface electrons orbital-selectively, suggesting different roles in SC and in AFM, and making orbital characters of the Fe magnetic moment resolvable by measuring the electronic structures. This work was supported by the NRF of Korea (Grant No. 2009-0081204). Computational resources have been provided by KISTI Supercomputing Center (Project No. KSC-2008-S02-0004)

Hyungju Oh
Department of Physics and IPAP, Yonsei University

Date submitted: 18 Nov 2010 Electronic form version 1.4