Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

A LDA+DMFT+Vertex function study of dynamical magnetic susceptibility in iron based superconductors HYOWON PARK, KRISTJAN HAULE, GABRIEL KOTLIAR, Rutgers University — We developed a method for computing dynamical magnetic susceptibility in complex correlated materials based on LDA+DMFT+Vertex function calculation. The dressed Greens function was obtained from the charge self-consistent LDA+DMFT calculation and the local Vertex function was computed from the quantum impurity model using a CTQMC impurity solver. We applied this method to compute the normal state magnetic susceptibility in iron pnictides and iron chalcogenides. Our result shows good agreement with inelastic neutron scattering data. At a low energy, the dynamical structure factor S(Q,w) is peaked at (π,0) momentum in $BaFe_2As_2$ and at ($\pi/2$,$\pi/2$) in FeTe, as expected for the distinct ordering of these compounds. At higher energy, the peak positions shifts to the (π,π) wave vector, in agreement with recent neutron experiments. We argue that this (π,π) magnetic response at high energy and the full spin dispersion above Neel temperature is captured by our realistic band structure method, LDA+DMFT.

Hyowon Park
Rutgers University

Date submitted: 19 Nov 2010 Electronic form version 1.4