MAR13-2012-020312

Abstract for an Invited Paper
for the MAR13 Meeting of
the American Physical Society

**Effects of disordered substitutions and vacancies in Fe based superconductors from first principles**[1]

TOM BERLIJN, University of Florida

Most Fe pnictide and selenide superconductors are created by chemical substitution which inevitably introduces disorder. The relationship between nominal chemical valence, doping, and quasiparticle spectral weight appears to be quite complex. Using a recently developed Wannier function based first principles method for disordered systems [1], we compute the configuration-averaged spectral function $\langle A(k,\omega)\rangle$ of Fe based superconductors containing disordered substitutions and vacancies. In the transition metal doped $Ba(Fe_{1-x}M_x)_2As_2$ with M=Co/Zn we find[2] a loss of coherent carrier spectral weight. For the case of disordered Fe and K vacancies in $K_{0.8}Fe_{1.6}Se_2$ we find a disorder induced effective doping to give rise to enlarged electron pockets without adding electrons to the system. For the case of Ru substitutions in $Ba(Fe_{1-x}Ru_x)_2As_2$ we find[4] a cancelation between on- and off-site disorder to give rise to a surprising protection of the Fermi surface.

[1] T. Berlijn, D. Volja and W. Ku, PRL 106, 077005 (2011)
[2] T. Berlijn, C.-H. Lin, W. Garber and W. Ku, PRL 108, 207003 (2012)
[3] T. Berlijn, P. J. Hirschfeld and W. Ku, PRL 109, 147003 (2012)
[4] L. Wang, T. Berlijn, Y. Wang, C.-H. Lin, P. J. Hirschfeld and W. Ku, arXiv:1209.3001

[1]Work supported by DOE CMCSN