Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Origin for the disorder-induced quantum criticality in $NbFe_2$[1]
AFTAB ALAM, DUANE JOHNSON, Division of Materials Science and Engineering, Ames Laboratory, Ames, Iowa — Using KKR-CPA ab-initio electronic-structure method founded on an optimal site-centered basis-set, we investigate the key features giving rise to the quantum critical transitions observed in $NbFe_2$ upon doping with 1.75% Nb [1]. These phase transitions involve lowest-energy excitations at/near the Fermi surface. In particular, it is suggested to arise due to an accidental unconventional band critical point (uBCP) with vanishing quasi-particle velocity [2]. Moving off-stoichiometry by increasing Nb, or reducing electrons (e/a), we find the Fermi level E_f increases (rather than decreases based only on band-filling) and meet the uBCP to produce excitations driving the anomalies. We detail the concentration-dependence electronic dispersion, density of state, E_f shift, and energies for $NbFe_2$, and why disorder increase the E_f with electron loss. At stoichiometry all our results agree with those from full potential calculations, including itinerant magnetism.

[1] D. Moroni-Klementowicz et al., Phys. Rev B 79, 224410 (2009).
[2] Brian Neal, Erik R. Ylviskar, and Warren E. Pickett, private communication (2009).

[1]Work was supported by the Department of Energy, Office of Basic Energy Science under contracts DE-FG02-03ER46026, as well as DE-AC02-07CH11358 at the Ames Laboratory operated by Iowa State University.

Aftab Alam
Division of Materials Science and Engineering,
Ames Laboratory, Ames, Iowa

Date submitted: 20 Dec 2010 Electronic form version 1.4