Origin for the disorder-induced quantum criticality in NbFe$_2$\textsuperscript{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.


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