Effects of Disordered Substitutions and Vacancies in Fe Based Superconductors from First Principles

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Using a recently developed Wannier function based first principles method [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 in addition to an increased chemical potential a loss of coherent carrier spectral weight [2]. For the case of isovalent substitutions we find the Fermi surface to be protected against the influence of disorder, surprisingly even in $Ba(Fe_{1-x}Ru_x)_2As_2$. For the case of disordered Fe and K vacancies in $K_{0.8}Fe_{1.6}Se_2$ we find a Fermi surface consisting of large/small electron pockets in the zone corners/center [3], in good agreement with ARPES measurements.

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[3] T. Berlijn, P. J. Hirschfeld, and W. Ku, arXiv:1204.2849.

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