One-Fe versus Two-Fe Brillouin Zone of Fe-Based Superconductors: Creation of the Electron Pockets via Translational Symmetry Breaking

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We investigate the physical effects of translational symmetry breaking in Fe-based high-temperature superconductors due to alternating anion positions [1]. In the representative parent compounds, including the newly discovered Fe-vacancy-ordered K$_{0.8}$Fe$_{1.6}$Se$_2$, an unusual change of orbital character is found across the one-Fe Brillouin zone upon unfolding the first-principles band structure and Fermi surfaces [2], suggesting that covering a larger one-Fe Brillouin zone is necessary in experiments. Most significantly, the electron pockets (critical to the magnetism and superconductivity) are found only created with the broken symmetry, advocating strongly its full inclusion in future studies, particularly on the debated nodal structures of the superconducting order parameter.


Work supported by DOE DE-AC02-98CH10886.

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Date submitted: 11 Nov 2011

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