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Symmetry breaking and Orbital fluctuation in iron pnictides

ZHIPING YIN, Department of Physics, UC Davis & Department of Physics, Rutgers University, WARREN PICKETT, Department of Physics, UC Davis — To perform a local orbital analysis of electronic and magnetic interactions, we construct Wannier functions of the Fe $3d$ orbitals in several parent compounds of the newly discovered iron pnictide superconductors in both nonmagnetic and antiferromagnetic phases, and use a tight binding representation to fit the DFT-LSDA Fe-derived bands. The calculated hopping parameters indicate that electrons in the Fe $3d_{xz}$ ($3d_{yz}$) orbital have a larger amplitude to hop in the y (x) direction rather than the x (y) direction. Weak stripe antiferromagnetism causes the spin-majority electron in Fe $3d_{xz}$ orbital hop in both x and y directions, but not so for the $3d_{yz}$ (possible because tetragonal symmetry is lost). This difference reinforces anisotropy which is accompanied by a large broken symmetry in the $3d_{xy}$ orbital. To take advantage of a kinetic energy gain from this additional hopping process, orbital fluctuation is favored, which reduces the ordered Fe magnetic moment in the stripe antiferromagnetic phase, consistent with experimental observations. It will also be shown how the pnictide atom is influential in forming the stripe antiferromagnetism. Interlayer hopping of Fe $3d$ electrons in the z direction may inhibit fluctuations and thereby help to stabilize the ordered magnetic moment of Fe in the stripe antiferromagnetic phase.

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