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Phase diagram of doped $BaFe_2As_2$ superconductor under broken C_4 symmetry YUAN-YEN TAI, Department of Physics, University of Houston, JIAN-XIN ZHU, MATTHIAS J. GRAF, Theoretical Division, Los Alamos National Laboratory, C.S. TING, Department of Physics, University of Houston, DEPARTMENT OF PHYSICS, UNIVERSITY OF HOUSTON TEAM, THEORETICAL DIVISION, LOS ALAMOS NATIONAL LABORATORY TEAM — We developed a minimal multi-orbital tight-binding model with realistic hopping parameters that breaks the symmetry of the point group by lowering it from C_4 to D_{2d}. The model accurately describes the Fermi surface evolution of the electron, $BaFe_{2-x}Co_xAs_2$, and hole, $Ba_{1-y}K_yFe_2As_2$, doped compounds. Since in this class of materials the competing superconductivity and co-linear antiferromagnetism rely on the evolution of the Fermi surface with doping, we investigated the phase diagram with a mean-field t-U-V Bogoliubov-de Gennes equation. Our results match the experimental electron-doped phase diagram. Furthermore, the model is in reasonable agreement with the experimental hole-doped part with only one set of t, U and V parameters. The self-consistently calculated superconducting order parameter exhibits s+/-d pairing symmetry in the entire doping range. It is the subtle result of competing interactions in the multi-orbital mean-field Hamiltonian based on the broken C_4 symmetry and might be observable in STM and ARPES experiments.

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