Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Phase diagram of doped BaFe$_2$As$_2$ superconductor under broken
C$_4$ symmetry

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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$_x$As$_2$,
and hole, Ba$_{1-y}$K$_y$Fe$_2$As$_2$, doped compounds. Since in this class of materials the
competing superconductivity and co-linear antiferromagnetism rely on the evolu-
tion 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 exper-
imental 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 ex-
hibits 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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Date submitted: 17 Nov 2012

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