Complex electronic structure of iron-based superconductors as a key to high temperature superconductivity

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The iron based superconductors (FeSC) promise interesting physics and applications, and, while the interplay of superconductivity and magnetism, as well as their mechanisms remain the issues of active debates and studies, one thing in FeSC puzzle is clear, namely that it is the complex multi-band electronic structure of these compounds that determines their rich and puzzling properties [1, 2]. What is important and fascinating is that this complexity seems to play a positive role in the struggle for understanding the FeSC physics and also for search of the materials with higher T_c's. This is because the multiple electronic bands and resulting complex Fermiology offer exceptionally rich playground for establishing useful empirical correlations. This is also because this electronic structure is well understood—the band structure calculations well reproduce its complexity: all the bands and their symmetry. The role of the experiment, in this case, is just to define the exact position and renormalization for each band. This piece of experimental knowledge, however, appears to be vitally important for understanding of the electronic properties of these new compounds.

Considering all the electronic band structures of FeSCs that can be derived from ARPES [3-7], it has been found that the Fermi surface of every optimally doped compound (the compounds with highest T_c) has the Van Hove singularities of the Fe $3d_{xz/yz}$ bands in the vicinity to the Fermi level. This suggests that the proximity to an electronic topological transition, known as Lifshitz transition, for one of the multiple Fermi surfaces makes the superconductivity dome at the phase diagram. Based on this empirical observation, one can predict, in particular, that the hole overdoping of KFe_2As_2 and LiFeAs compounds is a possible way to increase the T_c.

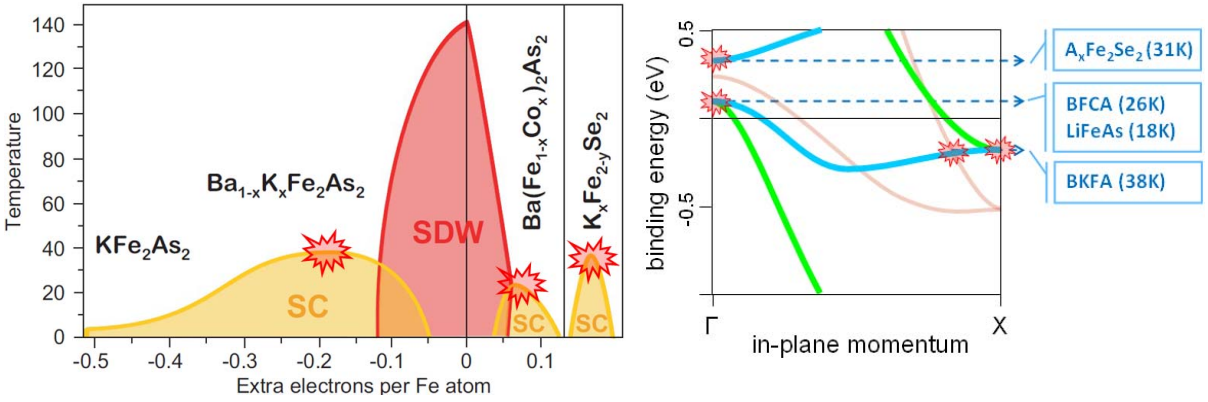

Figure 1. Phase diagram of the 122 family complemented by the 122(Se) family as a generalized band structure driven diagram for FeSCs (left) and common electronic band structure of the FeSCs (right): the compounds with highest T_c has either top or bottom of the Fe $3d_{xz/yz}$ bands crossing the Fermi level.

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