Electronic structure of iron based superconductors: pnictides versus chalcogenides and similar new systems

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We present a brief review of the present day situation with studies of electronic structure of new iron pnictide and chalcogenide high-temperature superconductors. Recent discovery of superconductivity with $T_c > 30$ in $A_xFe_{2-y}Se2$ (A=K,Cs,...) and possible observation superconductivity in single-layer FeSe up to 50 K represents the major new steps in the development of new concepts in the physics of Fe based high-temperature superconductors.

We compare LDA and ARPES data on the band structure and Fermi surfaces of novel $A_xFe_{2-y}Se_2$ and single-layer FeSe system and those of the previously studied isostructural 122 - superconductors like $BaFe_2As_2$ series. Electronic structure of new superconductors is rather different from that of FeAs - systems. In particular, no nesting properties of electron and hole - like Fermi surfaces is observed, casting doubts on some of the most popular theoretical schemes of Cooper pairing and magnetic ordering for these systems.

We discuss our recent results on correlated electronic structure of $K_{1-x}Fe_{2-y}Se_2$ (at different dopings) in the normal phase using the novel LDA'+DMFT computational approach. We show that this iron chalcogenide is more correlated in a sense of bandwidth renormalization (close enough to the Fermi level). Our results for spectral densities are in general agreement with recent ARPES data on this system. In general LDA'+DMFT results are in better agreement with experimental spectral function maps, as compared to the results of conventional LDA+DMFT.

We also present our results on electronic structure for several new systems like $BaFe_2Se_3$ (Ba123), $SrPt_2As_2$ and APt_3P (A=Cs, Sr, La).

Undoped Ba123 is antiferromagnetic with Neel temperature = 250K and rather complicated magnetic structure. Neutron diffraction experiments indicated the possibility of two possible spin structures (antiferromagnetically ordered "plaquettes" or "zigzags"), indistinguishable by neutron scattering. Using LSDA calculated exchange parameters we estimated Neel temperatures for both spin structures within the molecular field approximation and showed that "plaquettes" spin configuration is more favorable "zigzags".

Despite chemical and structural similarity of $SrPt_2As_2$ ($T_c = 5.2$K) to 122 FeAs-based high-temperature superconductors, its electronic structure is very much different. Fermi surface of $SrPt_2As_2$ is essentially three dimensional, with complicated sheets corresponding to multiple bands. Somehow similar situation is realized in APt_3P (A=Cs, Sr, La) system, which also demonstrates three-dimensional multiple band structure, with pretty complicated Fermi surface.

Finally, we address the general problem - which (if any) electronic structure is most favorable for high-temperature superconductivity?