High Temperature Superconductivity in an Iron Chalcogenide with a Very Simple Fermi-Surface

1) arXiv:1201.5694, by Q-Y Wang, Z. Li, W-H Zhang, Z-C Zhang, J-S Zhang, W. Li, H. Ding, Y-B Ou, P. Deng, K. Chang, J. Wen, C-L Song, K. He, J-F Jia, S-H Ji, Y. Wang, L. Wang, X. Chen, X. Ma, Q-K Xue

2) arXiv:1202.5849, by D. Liu, W. Zhang, D. Mou, J. He, Y-B Ou, Q-Y Wang, Z. Li, L. Wang, L. Zhao, S. He, Y. Peng, X. Liu, C. Chen, L. Yu, G. Liu, X. Dong, J. Zhang, C. Chen, Z. Xu, J. Hu, X. Chen, X. Ma, Q. Xue, X. J. Zhou

Recommended and a Commentary by Qimiao Si, Rice University

In early 2008, the condensed matter physics community greeted the news of superconductivity in doped LaFeAsO [1] with much excitement. The transition temperature T_c rapidly rose to about 55 K in related 1111 iron pnictides. There was also a sense that these systems will provide much new insights into unconventional superconductivity, because there is a large number of related materials to explore.

The latest development extends this materials parameter space into a new direction: Wang *et al.* reported evidence that one or a few layers of FeSe grown on an $SrTiO_3$ substrate superconduct, and T_c is at least as high as for most existing families of the iron pnictides and chalcogenides and may even be higher than 55 K. ARPES studies of Liu *et al.* provide evidence that this material has only two electron pockets on the Fermi-surface. This suggests, if as is reasonable that the fundamental physics of all the chalcogenides is the same, that it may be captured in a model with many fewer details than required to describe most of the other materials of this class. It also implies that Fermi-surface nesting does not have much to do with either antiferromagnetism or superconductivity in these compounds.

The bulk iron selenide ($\alpha-$FeSe) superconducts with a T_c slightly below 10 K (Ref. [2]). The Fermi surface is similar to that of the iron pnictides, containing both hole and electron pockets. Also like the pnictides, superconductivity in FeSe appears in its phase diagram near antiferromagnetism. The wavevector of the antiferromagnetic order, however, is $(\pi/2, \pi/2)$ (Refs. [3, 4]), instead of $(\pi, 0)$ for the pnictides, suggesting a diversity in the relationship between Fermi surfaces and antiferromagnetism.

Late 2010 saw the discovery of superconductivity in the alkaline iron selenides, $K_{1-y}Fe_{2-x}Se_2$, whose parent compounds are Mott insulators. Superconductivity arises with a doping concentration of about

0.2 electrons/Fe, and T_c is as high as for the optimally doped 122 iron pnictides such as $\mathrm{Ba(Fe_{1-x}Co_x)_2As_2}$. Yet, the Fermi surface contains only electron pockets. For a perspective, see the July 2011 issue of JCCM.

In the new planar FeSe structure, ARPES (Liu *et al.*) shows that, here too, the Fermi surface comprises only electron pockets. (A layer of FeSe is defined in terms of an Fe plane sandwiched by two Se planes.) It is in fact the simplest, with two electron pockets located at the edges of the Brillouin zone for the Fe square lattice.

The mechanism for iron based superconductors remains a subject of debate. Two approaches have been particularly prominent. A weak-coupling picture studies the electron interactions as a perturbation, and invokes the nesting between hole and electron pockets to understand antiferromagnetism and superconductivity. A strong-coupling picture treats the metallic regime of the iron based materials as in proximity to a Mott insulator, and considers the associated short-range exchange interactions as driving both the antiferromagnetism and superconductivity.

Nesting between hole and electron pockets refers to the enhancement such dispersions generate in the response of quasiparticles in the spin and related particle-hole channels. It does not operate between two purely electron pockets. Correspondingly, the fact that T_c is high in the new planar FeSe systems is at odds with the weak-coupling nesting description. The new results instead provide evidence for the strong-coupling approach.

The new development also brings out some welcome simplifications to the theoretical studies of the iron based superconductors. The simplicity of the Fermi surface makes likely a simplified parameterization of the electronic structure. Furthermore, the results suggest that superconductivity in all the iron based compounds can be (adequately) understood by focusing on the electronic structure and correlations in two dimensions. The out-of-plane couplings, while important for establishing antiferromagnetic order at nonzero temperatures, may not be essential for superconductivity.

As exciting as these results and implications are, it is important to emphasize that studies on these planar FeSe structures are just beginning. There are many open questions to be addressed:

- Evidence for superconductivity has been provided by transport, STM and ARPES studies. Transport results have so far been reported only in a five-layer FeSe structure, identifying a zero-resistance temperature of about 30 K and superconducting onset temperature of 53 K. In the single-layer case, there is not yet any resistivity measurement, but STM (Wang *et al.*) has identified superconducting vortices in the presence of a magnetic field.

STM studies in the single-layer system have furthermore observed a gap that is consistent with superconductivity. The gap is very large – about 20 meV, which is nine times that of bulk FeSe. This has fueled speculation that T_c could be higher than the liquid nitrogen temperature. A similar gap has also been observed in ARPES.

Future experiments are needed to establish whether the observed gaps represent pseudogaps (which would be a very important result in its own right) or mark genuine superconductivity.

- ARPES shows that the single-layer system is doped by about 0.09 electrons/Fe. Where does the electron doping come from remains to be understood, with possibilities including the substrate or Se vacancies. In this connection, it is interesting to note that, in the case of several layers of FeSe, STM studies suggest that superconductivity is confined to the bottom layer (*i.e.*, the one closest to the substrate).
- In the bulk materials, superconductivity in FeSe borders on antiferromagnetism, which can be accessed by using Te to substitute Se. It will be very important to clarify whether this remains to be the case in the planar structures. For instance, does a single-layer FeTe grown on the same $SrTiO_3$ substrate orders antiferromagnetically at zero temperature?

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[1] Y. Kamihara et al., J. Am. Chem. Soc. **130**, 3296 (2008).

[2] F.-C. Hsu et al., PNAS **105**, 14262 (2008).

[3] W. Bao et al., Phys. Rev. Lett. **102**, 247001 (2009).

[4] S. Li et al., Phys. Rev. B **79**, 054503 (2009).