Iron Pnictides research coming of age

1. **Specific heat Measurements:** "Fully gapped superconducting state based on a high normal state quasiparticle density of states in $Ba_{0.6}K_{0.4}Fe_2As_2$ single crystals," G. Mu, H. Luo, Z. Wang, L. Shan, C. Ren and H.H. Wen.
   arXiv:0808.2941.

2. **ARPES Measurements:**"Observation of Fermi surface-dependent nodeless superconducting gaps in $Ba_{0.6}K_{0.4}Fe_2As_2$," H. Ding, P. Richard, K. Nakayama, K. Sugawara, T. Arakane, Y. Sekiba, A. Takayama, S. Souma, T. Sato, T. Takahashi, Z. Wang, X. Dai, Z. Fang, G.F. Chen, J.L. Luo, and N.L. Wang.
   arXiv:0807.0419, Europhys. Lett. **83**, 4701 (2008).

   "Unexpected Fermi surface topology in the new pnictide superconductor," V.B. Zabolotnyy, D.S. Inosov, D.V. Evtushinsky, A. Koitzsch, A.A. Kordyuk, J.T. Park, D. Haug, V. Hinkov, A.V. Boris, D.L. Sun, G.L. Sun, C.T. Lin, B. Keimer, M. Knupfer, B. Buechner, A. Varykhalov, R. Follath, and S.V. Borisenko, arXiv:0808.2454.

   "Tightly-bound Cooper pair, quasiparticle kinks and clues on the pairing potential in a high T_c FeAs Superconductor," L. Wray, D. Qian, D. Hsieh, Y. Xia, L. Li, J.G. Checkelsky, A. Pasupathy, K.K. Gomes, A.V. Vedorov, G.F. Chen, J.L. Luo, A. Yazdani, N.P. Ong, N.L. Wang, and M.Z. Hasan.
   arXiv:0808.2185.

3. **NMR on LaFePO**: "Spin dynamics in iron based layered superconductor $(La_{0.87}Ca_{0.13})FePO$ revealed by ^{31}P and ^{139}La NMR studies," Y. Nakai, K. Ishida, Y. Kamihara, M. Hirano, and H. Hosono.
   arXiv:0808.2293.

Recommended with a Commentary by Patrick Lee, MIT

The discovery of "higher T_c" in Fe pnictides this spring has taken the community by storm. One normally associates iron with ferromagnetism, making it the last place one might look for superconductivity. Yet Nature once again obliges us with a surprise gift which points to additional

pathways to high T_c superconductivity other than the cuprates. Early data invite obvious comparison with the cuprates: superconductivity in both cases arises from doping of a parent compound with antiferromagnetic order. However, the similarity stops there. Unlike the cuprate whose parent compound is a Mott insulator, the FeAs system has an even number of carriers per unit cell and starts out as a metal with small electron and hole pockets. The antiferromagnetic order is a spin density wave, probably due to nesting of these pockets. Unlike the cuprate where a single Cu $d_{x^2-y^2}$ orbital is active, the iron system involves multiple orbitals at the Fermi level. The key question is how strong is the correlation. Is the parent compound sufficiently close to a correlation driven insulator that one should start with a local moment description of the iron ion, or does an itinerant picture suffice? What is the role of Hund's rule coupling which is absent in the cuprates? Finally, what is the pairing symmetry?

To address the question of correlation one would like to have information on basic questions such as the size of γ (the coefficient of the linear T term in specific heat) which one can compare with band calculations to get an idea of the mass enhancement. Unfortunately, this is not an easy measurement to make, because superconductivity intervenes. Early data on polycrystalline samples did not give us a clue because the transition is very much smeared. Spin susceptibility data are also problematic because the early data are often dominated by local moment contributions. A few months ago a modification of the original structure LaFeAsO was discovered, where the LaO layer is replaced by a Ba layer which can be doped by K, resulting in the chemical formula $Ba_{1-x}K_xFe_2As_2$ (called the 122 material). Unlike the original $LaFeAsO_{1-x}F_x$ (1111 material), large single crystals of the 122 material can be made. Note that while the two materials share the same active FeAs layer, this 122 compound is hole doped while the original 1111 is electron doped. (In another version of 122, doping is accomplished by substituting Co for Fe in the FeAs plane, resulting in $BaFe_{2-x}Co_xAs_2$. This version is electron doped but has substantial in-plane disorder.) Recently a large number of experiments were performed on the 122 $Ba_{1-x}K_xFe_2As_2$ crystals. These include a specific heat experiment and three ARPES measurements selected here. The specific heat measurement by Mu *et al.* is particularly impressive in that for the first time a BCS-like jump in the specific heat is clearly observed at T_c (36 K). The jump is surprisingly large, ≈ 49 mJ/Fe-mol K^2. (I convert from the unit used in the paper mJ/mol K^2 to per Fe-mol for ease of comparison later.) The authors also measure a downward shift of T_c in a magnetic field up to 9 T, from which they extrapolate to obtain $H_{c2}(T = 0) = 100$ T. Using this value of H_{c2} they estimated $\gamma = 31.6$ mJ/Fe-mol K^2, which is consistent with the specific heat jump according to

the usual BCS ratio.

The γ value is very large compared with 6.5 mJ/Fe-mol K^2 obtained from LDA calculations for the undoped LaFeAsO.[1] Since the FeAs layer is basically unchanged, this is a reasonable starting point for comparison with the 122 material. Does this imply a mass enhancement of 5 and therefore strong correlation? I think this conclusion is unwarranted in light of several ARPES experiments done on the same 122 material. The consensus seems to be that overall the bands pretty much follow the LDA dispersion but with a factor of 2 band narrowing. Wray *et al.* directly measured the Fermi velocity of the inner hole pocket to be 0.7 eVÅ. Using the measured areas of the inner and outer hole pockets and assuming they have the same Fermi velocity, I estimate that the two hole pockets account for a γ of 6 mJ/Fe-mol K^2. Since the LDA calculation included the contributions from two electron pockets as well, these numbers are consistent with roughly a factor 2 renormalization of the Fermi velocity, not a factor 5. The question is then where do the remaining 30 mJ/Fe-mol K^2 come from. The paper by Zabolotnyy *et al.* found that the pockets near the M points are totally different from those predicted by LDA band calculations. Instead of roughly circular electron pockets they found elongated hole pockets which they call propeller blades. The band bottom of these blades is only about 20 meV below the Fermi level. Thus it is possible that a large part of the disagreement with the LDA γ value comes from band structure effects, and it will be interesting to see if the complicated low energy band near the M point has a large enough density of states to account for the very large observed γ. This will be consistent with the suggestion of Mu *et al.* that the γ for hole doped 122 materials may be 3 to 5 times larger than the electron doped 1111 compounds.

One interesting consequence of the low Fermi velocity noted by Wray *et al.* is that the standard formula $\xi_0 = v_F/\pi\Delta_0$ implies a surprisingly small ξ_0 of 20 Å or less, making it comparable to that of the cuprates, despite a much smaller energy gap. (This is because v_F for the cuprate is larger, ≈ 1.65 eVÅ.) The short coherence length gives $H_{c2}(0) = \phi_0/2\pi\xi_0^2 \approx 100$ T, consistent with that inferred from the specific heat data. Mu *et al.* also found that the H_{c2} anisotropy is modest. Together with the high $H_{c2}(0)$, this is good news for potential applications.

I end with a few comments about the issue of gap nodes. The ARPES paper by Ding *et al.* reported roughly isotropic gaps. The specific heat data at low temperatures is fitted by a gap of 6 meV, consistent with the smaller of the two gaps seen by ARPES, suggesting that these are bulk properties. Furthermore, the specific heat is linear in H, in contrast with the $\sqrt{H}$ behavior

measured by the same group on electron doped 1111 polycrystals earlier.[2] The latter was taken as evidence for nodes. Another strong evidence for nodes came from NMR measurement of $\frac{1}{T_1}$ in 1111 material, which fits T^3 law over almost 3 decades.[3] Thus, while the evidence is strong for the absence of gap nodes in the hole doped 122 material, the possibility that electron doped materials may be different remains open.

Finally, there is evidence that the Fe pnictides as a class may exhibit even more diverse behavior. A recent NMR paper on the original doped LaFePO material ($T_c \sim 8$ K) by Nakai *et al.* showed that its fundamental properties may be totally different. In the FeAs system, the Knight shift decreases by about a factor of two from room temperature to T_c. That in itself is a mystery. In FeP the Knight shift increases with decreasing temperature, suggestive of ferromagnetic fluctuations. Furthermore, its $\frac{1}{T_1 T}$ *increases* below T_c. I have not encountered this behavior in superconductors before and it seems hard to reconcile with spin singlet pairing. On the other hand, singlet pairing is quite well established on the electron doped 122 single crystal $BaFe_{2-x}Co_xAs_2$ by a Knight shift measurement.[4]

The availability of large single crystals has launched a new phase in the iron pnictide research. However, as is often the case in this line of work, it appears that things will get more complicated before they become simple.

---

[1] D.J. Singh and M. Du, Phys. Rev. Lett. **100**, 237003 (2008).

[2] G. Mu, X.-Y. Zhu, L. Fang, L. Shan, C. Ren, and H.-H. Wen, Chinese Phys. Lett. **25**, 2221 (2008).

[3] Y. Nakai, K. Ishida, Y. Kamihara, M. Hirano, and H. Hosono, J. Phys. Soc. Japan **77**, 073701 (2008).

[4] F.L. Ning, K. Ahilan, T. Imai, A. Sefat, R. Jin, M. McGuire, B. Sales, and D. Maudrus, J. Phys. Soc. Japan **77**, 103705 (2008).