(Tl,K)Fe$_{x}$Se$_2$

Iron-based Superconductors: Parent Antiferromagnet goes Insulating.

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Outline

- High-$T_C$'s: Cuprates vs. Pnictides
- Mott Insulators & High-$T_C$ Theory
- Parent Compounds of Pnictides
- $(Tl,K)Fe_2Se_2$: Similarities & Differences
- New Insights from these compounds
- Where to go from here...
High-$T_C$'s

- Generally defined as anything with a SC $T_C > 30K$.

- Two major families:
  - Cuprates (max. $T_C = 135K$)
  - Pnictides (max. $T_C = 56K$)
Cuprates vs. Pnictides

• Several families of both exist.
• They share many commonalities, including layering structure, proximity to magnetism, etc.
• Both require doping of the parent compounds, and superconduct with both hole- and electron-doping.
**Cuprates vs. Pnictides**

Keimer *et al.* PRB **46** (1992) **14034**

Ni *et al.* PRB **82** (2010) **024519**
Mott Insulators

- Mott insulators are materials which are insulating, despite being metals by band theory.
- This is due to large electron-electron interactions.
- Large $U$ repulsion localizes the electrons, creating a band gap.
Cuprates as doped Mott Insulators

Keimer et al. PRB 46 (1992) 14034

- One view of high-TC SC is that they arise from AF Mott insulators.
Parent Compounds

- In the parent materials of 1111s (e.g. LaFeAsO) and 122s (e.g. BaFe$_2$As$_2$), as well as others, they are reasonably good metals.

- They do display AF, and it has been speculated that they may be close to a Mott transition.

- Increasing $U/t$ may push it through the Mott transition, e.g. La$_2$O$_3$Fe$_2$Se$_2$. 
La$_2$O$_3$Fe$_2$Se$_2$

- Expanded unit cell.
- Band narrowing compared to LaFeAsO.

Zhu et al. PRL 104 (2010) 216405
\((\text{Ti, K})\text{Fe}_2\text{Se}_2\)

- Similar phase diagram, except insulating at low dopings.
- Still a modest \(T_c = 31\text{K}\).
- Most properties are independent of K doping.
\((\text{Tl,K})\text{Fe}_2\text{Se}_2\)

- Resistivity shows several orders of magnitude change with Fe-doping.
- Kink seen at \(T_N\).
- Sharp SC transition.
\[(\text{Tl,K})\text{Fe}_2\text{Se}_2\]

- Similar phase diagram, except insulating at low dopings.
- There is still an overlap between AF and SC states.
- The interesting difference is in the Fe content.
Iron Deficiencies

- AF insulating behaviour only occurs with Fe vacancies.
- This may be due to ordering of the vacancies.
Iron Deficiencies

- A large change is seen in $R_H$ with changing Fe doping, but no change with K doping.
- Shows abrupt changes in carrier concentration at $T_N$ and $T_C$. 
Are they Mott Insulators?

- As with $\text{La}_2\text{O}_3\text{Fe}_2\text{Se}_2$, this material has a larger Fe-Fe spacing, hence a lower kinetic energy, $t$.

- Enhancing $U/t$ turns the material into a Mott insulator.

- In $(\text{Tl,K})\text{Fe}_{2-x}\text{Se}_2$, with $x=0.4$, NS found a nominal Fe valence of 2+, and $m_\text{Fe} \approx 3\mu_\text{B}$. 
Are they Mott Insulators?

- It seems that the parent compounds of $A\text{Fe}_{2-x}\text{Se}_2$ are naturally described as Mott insulators.
  - The enhanced $U/t$ from the Fe vacancies push it through the Mott transition.
- There is evidence of strong electron-electron coupling (LDA) and an integer number of electrons in the Fe $3d$ orbitals.
  - Falls in line with a Mott insulator.
What's next?

- Studies on potential vacancy ordering may illustrate microscopic properties.
- With doping, we may be able to access a metal-insulator transition.
- Most importantly, it may help to illustrate Mott physics and its role in superconductivity.
See you next week!