Iron-Chalcogenide Superconductors
Outline

Fe-chalcogenides vs. Fe-pnictides
Electronic structure calculations of undoped chalcogenides
Spin-density wave?
FeSe
FeTe
Electronic structure calculations of doped FeTe
Conclusion
LaFeAsO$_{1-x}$F$_x$ ($T_c = 26$ K)
SmFeAsO$_{1-x}$F$_x$ ($T_c = 55$ K)
LaFeAs$_{1-x}$Sb$_x$O$_{1-x}$F$_x$ ($T_c = 29$ K)
Ba$_{1-x}$K$_x$Fe$_2$As$_2$ ($T_c = 38$ K)
Sr$_{1-x}$K$_x$Fe$_2$As$_2$ ($T_c = 32$ K)
Li$_{1-x}$FeAs ($T_c = 18$ K)

FeSe$_{1-x}$ ($T_c = 8$ K)
FeTe$_{1-x}$S$_x$ ($T_c = 10$ K)
FeSe$_{0.5}$Te$_{0.5}$ ($T_c = 15$ K)
Many Similarities

Common square planar sheets of tetrahedrally coordinated Fe$^{2+}$

Neither can be understood in terms of standard el-ph theory

Fermi surface nesting whose nesting vector corresponds to the AFM ordering vector

Low carrier density, high DOS

Very similar band structures
Chalcogen vs. Pnictogen

Magnetic ordering observed experimentally is very different

Recent electronic structure calculations reveal topological differences

Fe-chalcogenides have the simplest crystal structure among Fe-based SCs

Fe-chalcogenides nontoxic
Fe $d$ states dominate Fermi level

$E_f$ lies near bottom of a pseudogap

Spin-Density Wave

First seen in Cr

AFM ground state for which the density of conduction-electron spins is spatially modulated

Occurs at low T in anisotropic metals with large DOS at Fermi level so that a single nesting vector $Q$ can map large areas of Fermi surface onto another

Development of a SDW causes modulation in the spin density with periodicity of $2\pi/Q$

The spatial modulation leads to a lowering of the energy, which opens an energy gap at the Fermi level

Condensation energy $\sim N(E_f)\Delta$

Half-filled band case (AFM) satisfies nesting vector $\mathbf{Q} = (\pi, \pi)$

Susceptibility $\chi(\mathbf{q})$ diverges at nesting vector

$$\chi(\mathbf{q}) = \sum_{\mathbf{k}} \frac{f_{\mathbf{k}} - f_{\mathbf{k}+\mathbf{q}}}{\varepsilon_{\mathbf{k}+\mathbf{q}} - \varepsilon_{\mathbf{k}}}$$
Similarly sized cylinders yield strong nesting at $(\pi, \pi)$ point.

FeSe

PbO-type structure (tet)
Structural phase transition at 70 K
Clean SC phase observed only in Se-deficient (?) FeSe

At 105 K, tet (P4/nmm) → triclinic (P-1)

SC transition very broad
Doesn't follow BCS at lower T
Stoichiometric FeTe not superconducting

Tet → ortho at 80 K

Structural phase transitions (tet → ortho)

FeTe$_{0.92}$: 80 K

FeTe$_{0.9}$S$_{0.1}$: < 50 K

FeTe$_{0.8}$S$_{0.2}$: none

Nesting reduced via doping, pressurization

Suppression of phase transition key to produce SC

Neutron scattering reveals double-stripe AFM ordering

Fe-doped calculations support this ordering

Double-stripe AFM ordering realized at $x \sim 0.068$ (~0.5 e-/u.c.)

Spin ordering becomes incommensurate at $x \sim 0.141$

$\langle \text{FeTe} \rangle$

$\langle \text{Fe}_{1+x} \text{Te} \rangle$

$(\pi, 0)$ nesting appears upon doping

$(\pi, \pi)$ nesting suppressed
Te $p$-bands hybridize with Fe $d$-bands

Band crossing observed near Fermi level

No band crossing across $X$

Mechanism for SC in Fe-based materials not fully established, but spin fluctuations may be associated with it.

Chemical doping and pressurization can raise Tc.

Clear association between SC and suppression of SDWs.

Little Fe doping affects magnetic structure significantly.

More study required to better understand systems.