Iron-Chalcogenide Superconductors

HB Rhee
Phy 242
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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)

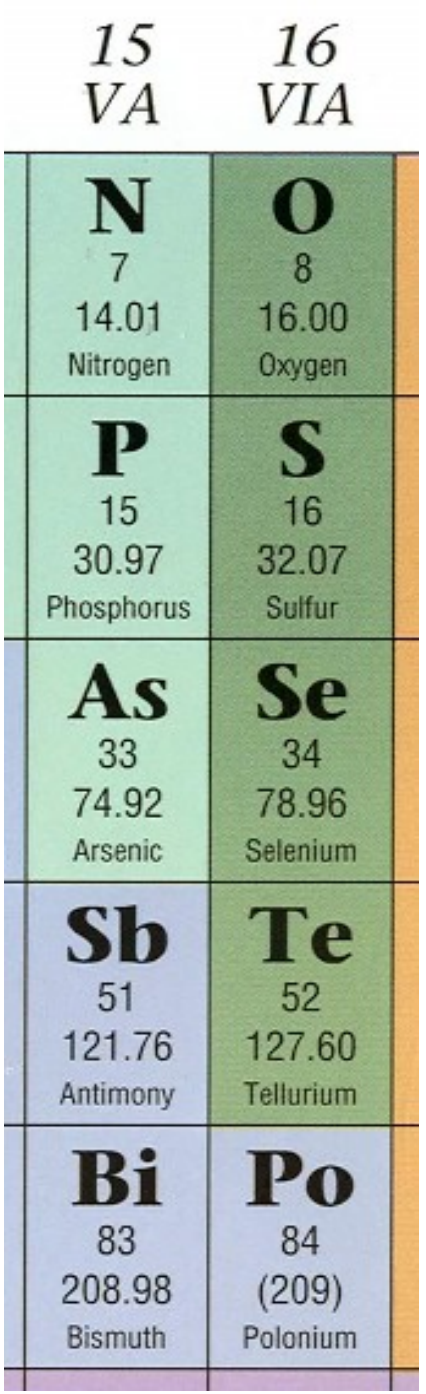
$SmFeAsO_{1-x}F_x$ (T_c = 55 K)

$LaFeAs_{1-x}Sb_xO_{1-x}F_x$ (T_c = 29 K)

$Ba_{1-x}K_xFe_2As_2$ (T_c = 38 K)

$Sr_{1-x}K_xFe_2As_2$ (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

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

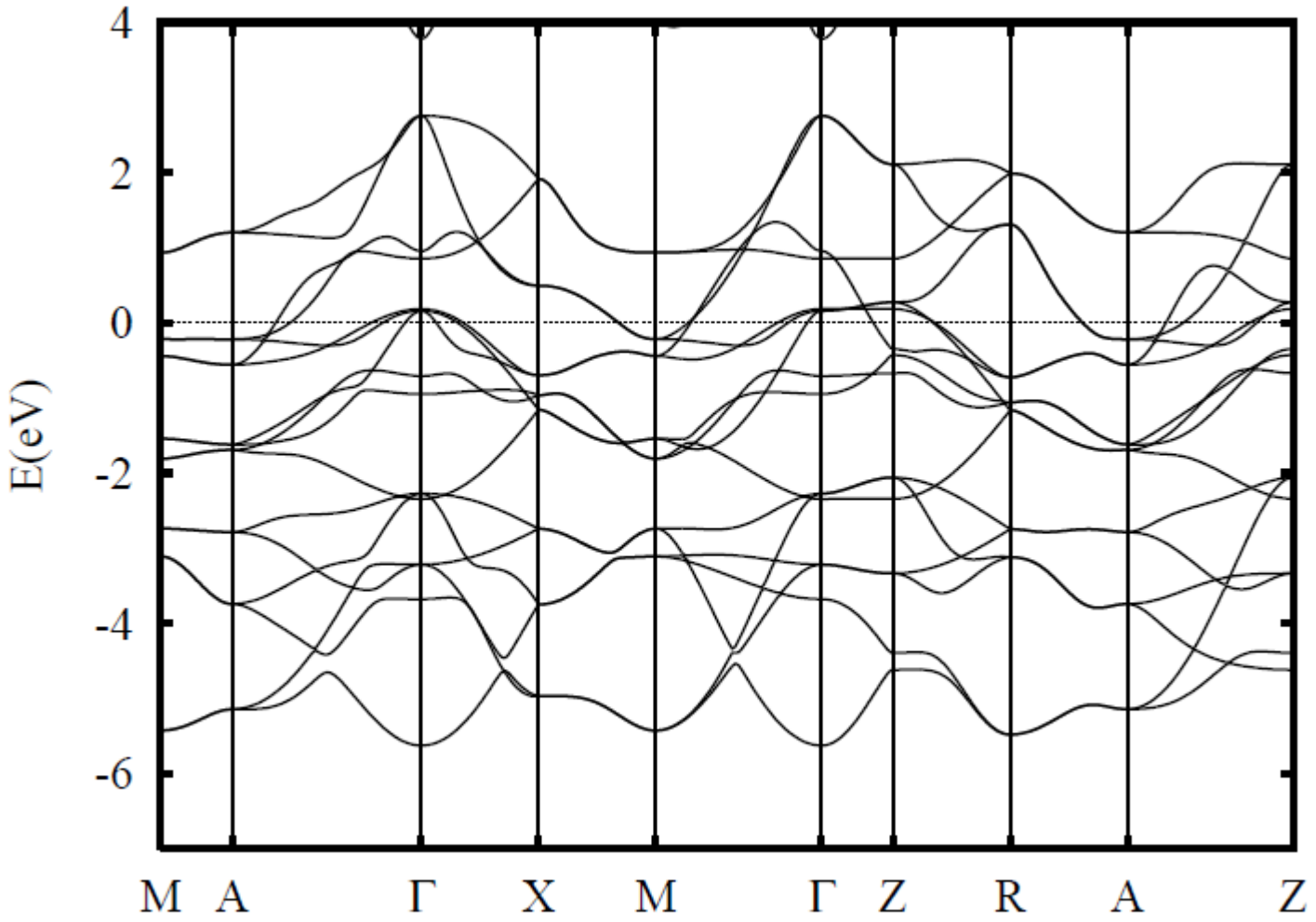
Chalcogen vs. Pnictogen

Magnetic ordering observed experimentally is very different

Recent electronic structure calculations reveal topological differences

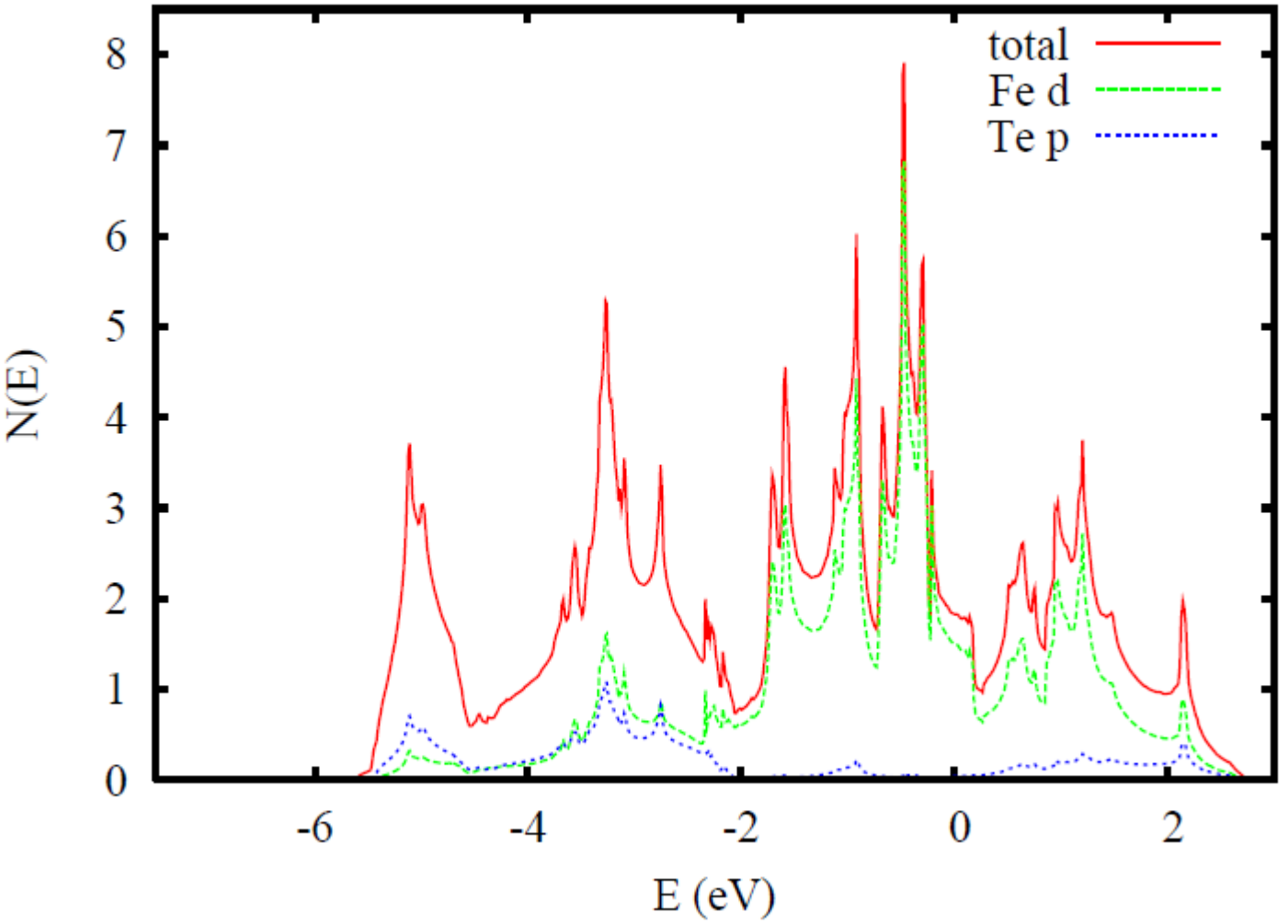
Fe-chalcogenides have the simplest crystal structure among Fe-based SCs

Fe-chalcogenides nontoxic



A. Subedi *et al.*, Phys. Rev. B **78**, 134514 (2008)

Undoped FeS, FeSe, FeTe



Fe *d* states dominate Fermi level

E_f lies near bottom of a pseudogap

A. Subedi *et al.*, Phys. Rev. B **78**, 134514 (2008)

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 $\sim N(E_f)\Delta$

A. W. Overhauser, Phys. Rev. **128**, 1437 (1962)

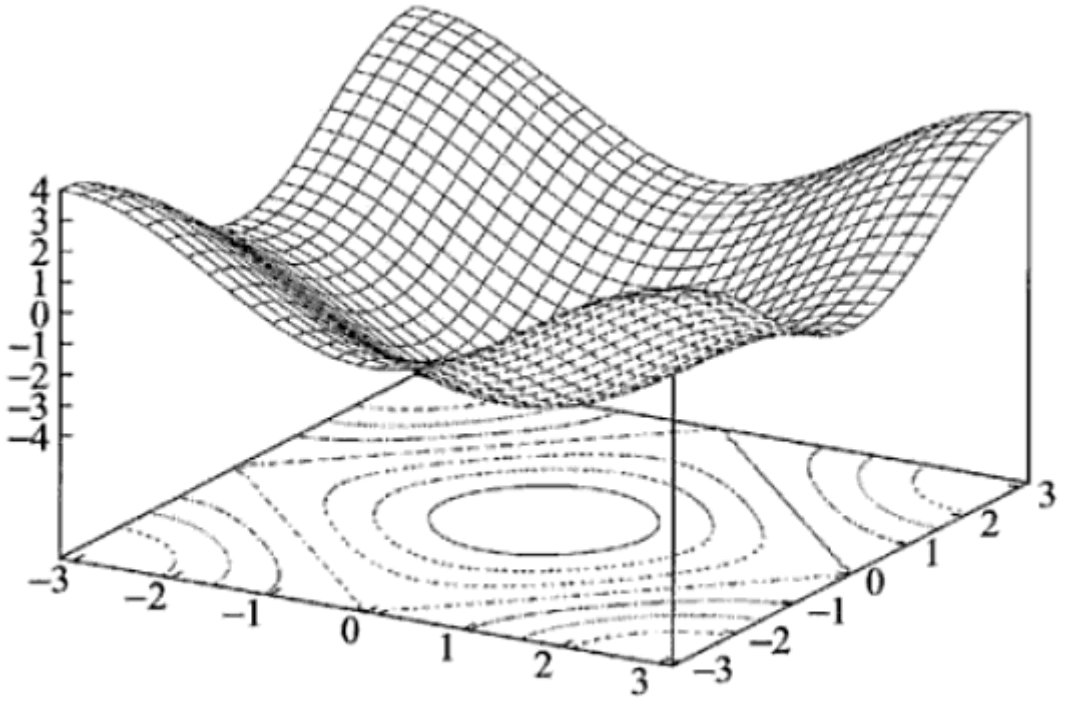
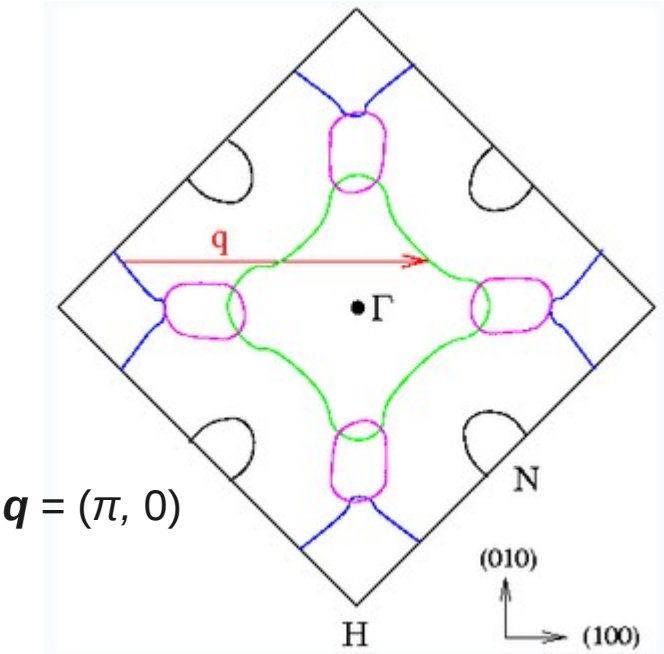


FIG. 5.17. The electron dispersion ξ_k in the Hubbard model.

$$H = -\sum_{\langle ij\rangle,\alpha} t(c^{\dagger}_{\alpha j} c_{\alpha i} + h.c.) + U\sum_{i} n_i^2$$

$$\xi_{\boldsymbol{k}} = -2t\left(\cos(k_x) + \cos(k_y)\right)$$



$\boldsymbol{q} = (\pi, 0)$

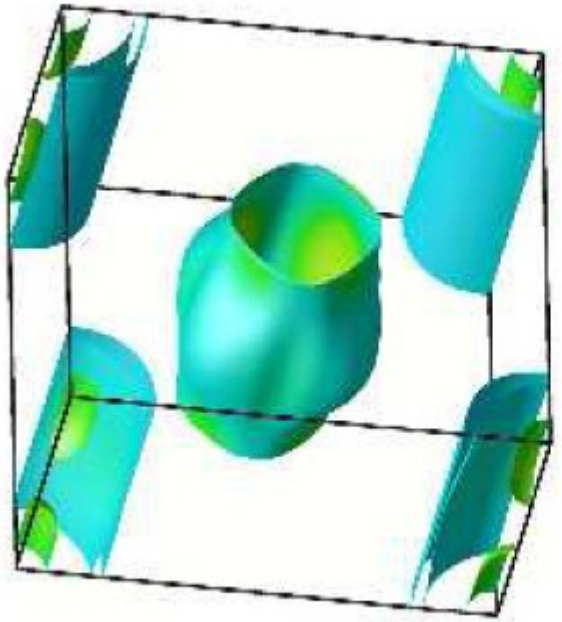
<FS of Cr>

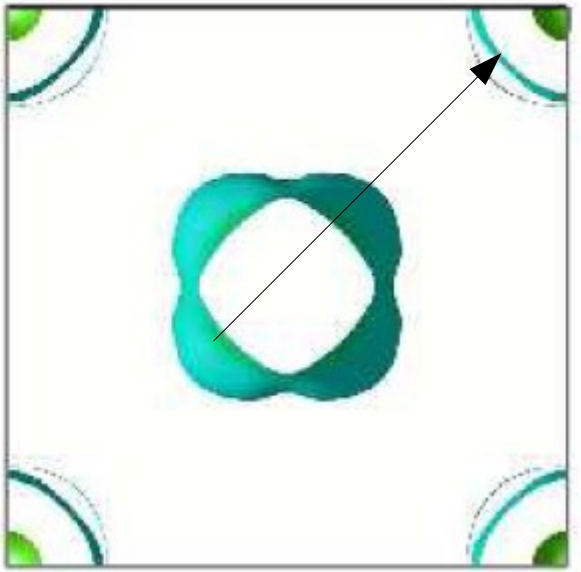
Half-filled band case (AFM) satisfies nesting vector $\boldsymbol{Q} = (\pi, \pi)$

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

$$\chi(\boldsymbol{q}) = \sum_{\boldsymbol{k}} \frac{f_{\boldsymbol{k}} - f_{\boldsymbol{k}+\boldsymbol{q}}}{\varepsilon_{\boldsymbol{k}+\boldsymbol{q}} - \varepsilon_{\boldsymbol{k}}}$$

FeTe

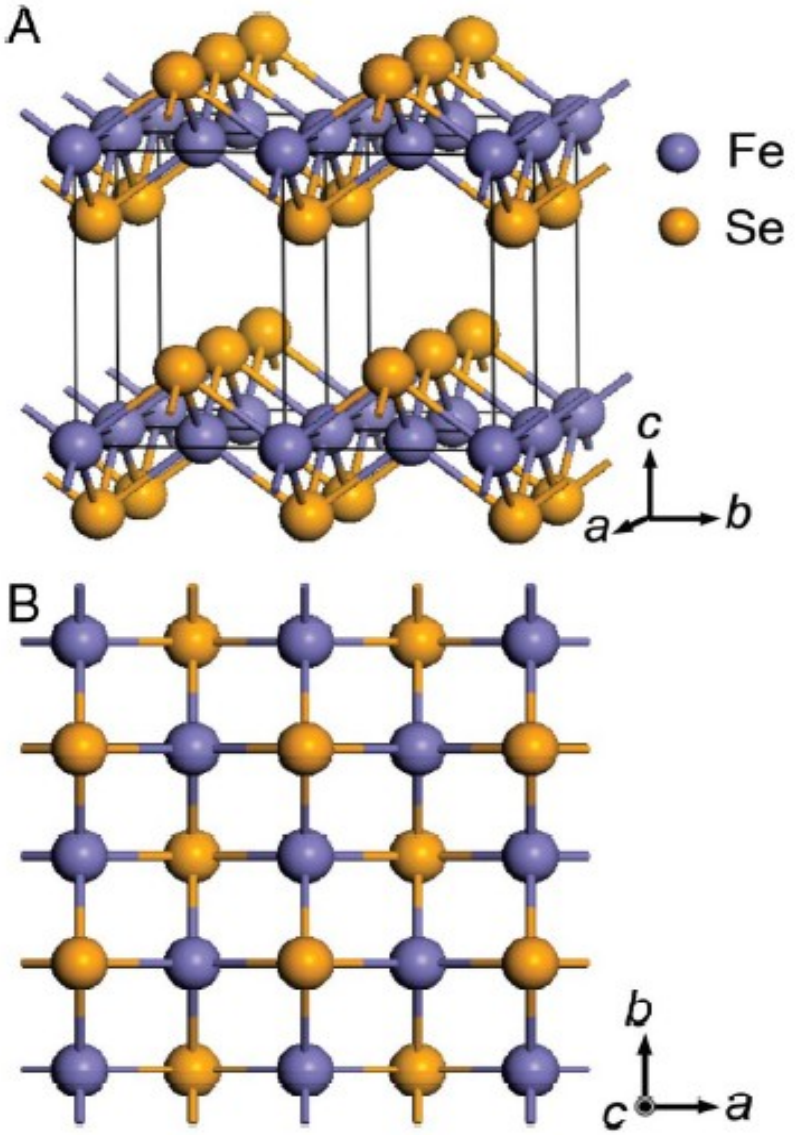




Similarly sized cylinders yield strong nesting at (π,π) point

A. Subedi *et al.*, arXiv:0807.4312v2 (2008)

FeSe

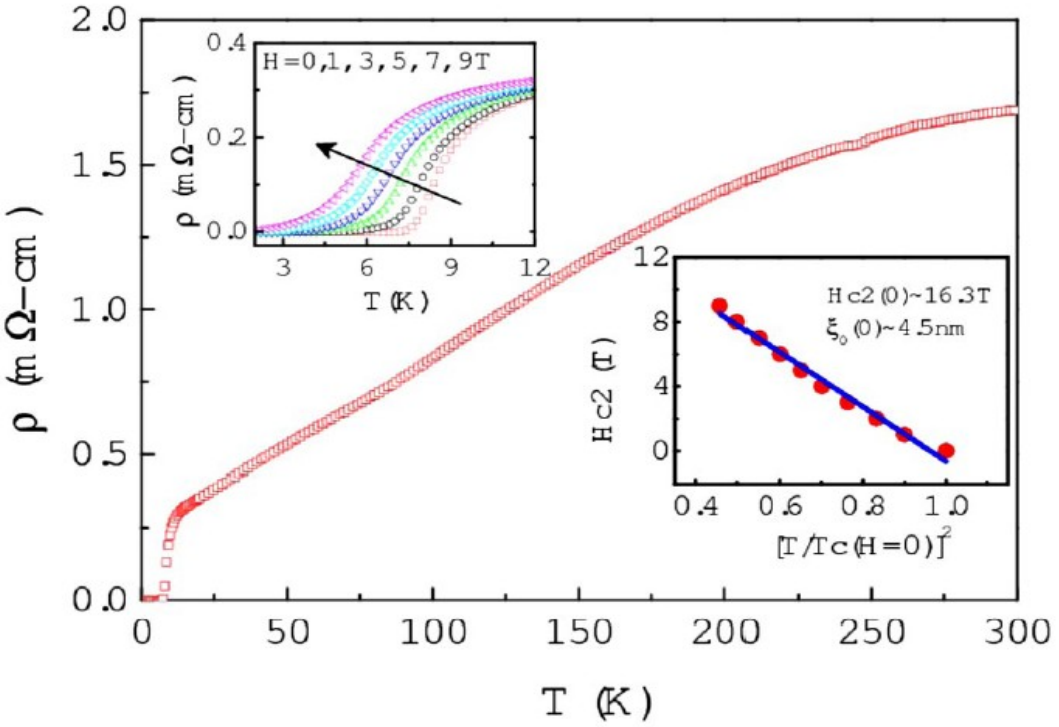


PbO-type structure (tet)

Structural phase transition at 70 K

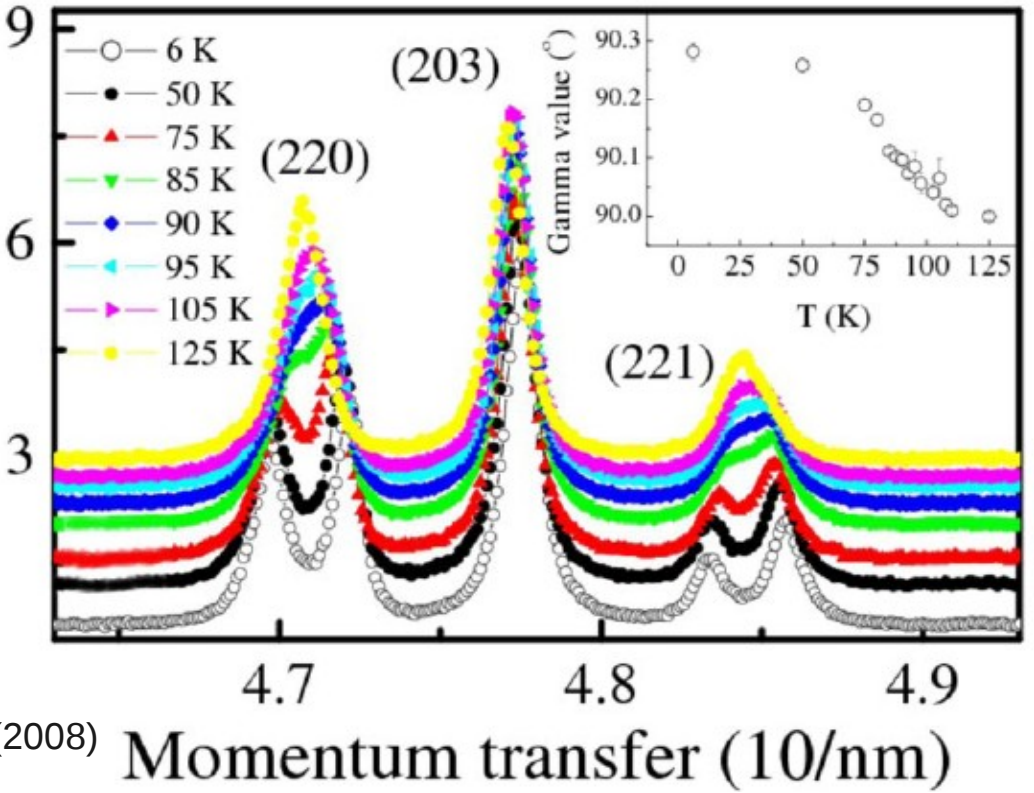
Clean SC phase observed only in Se-deficient (?) FeSe

F. C. Hsu *et al.*, Proc. Natl. Acad. Sci. U.S.A. **105**, 14262 (2008)

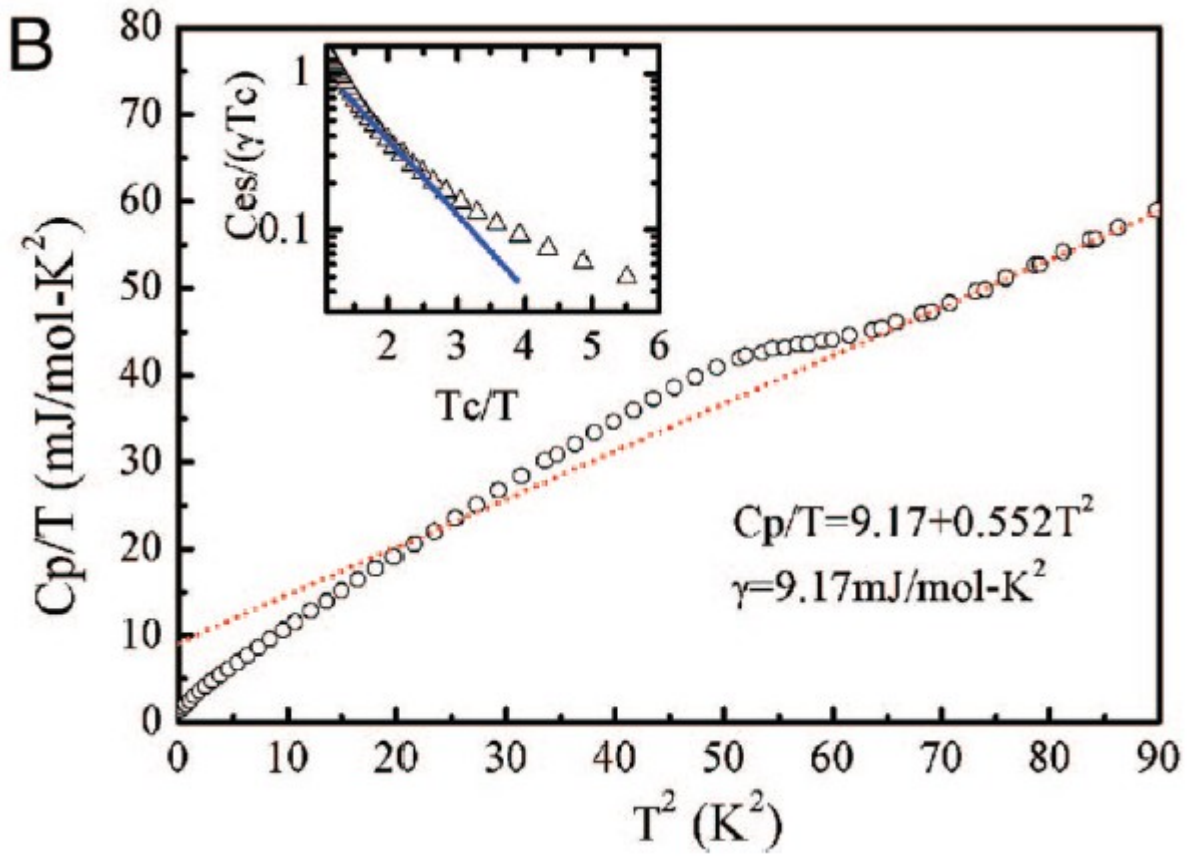


$FeSe_{0.88}$

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



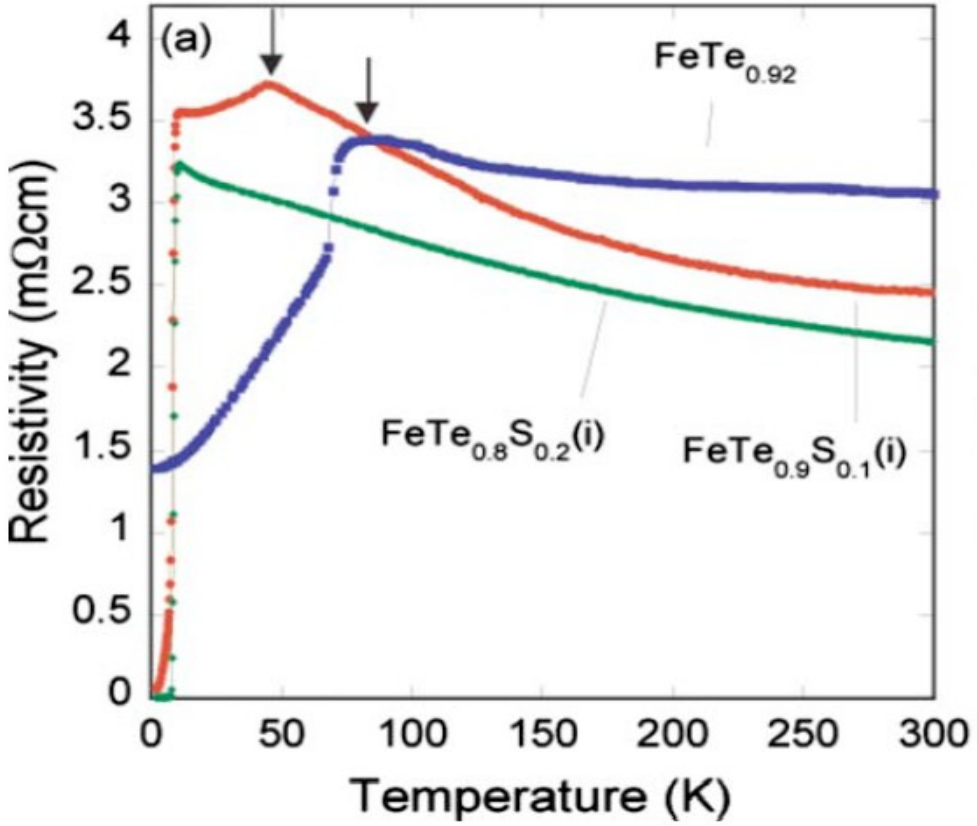
F. C. Hsu *et al.*, Proc. Natl. Acad. Sci. U.S.A. **105**, 14262 (2008)

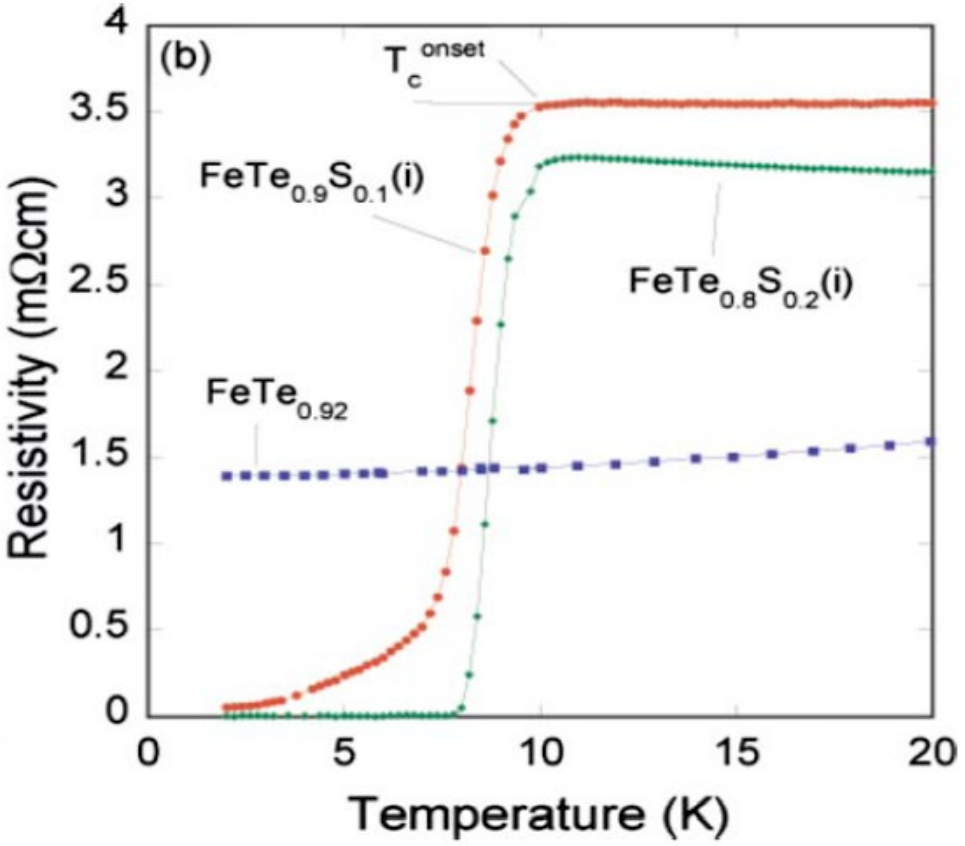


SC transition very broad

Doesn't follow BCS at lower T

F. C. Hsu *et al.*, Proc. Natl. Acad. Sci. U.S.A. **105**, 14262 (2008)





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

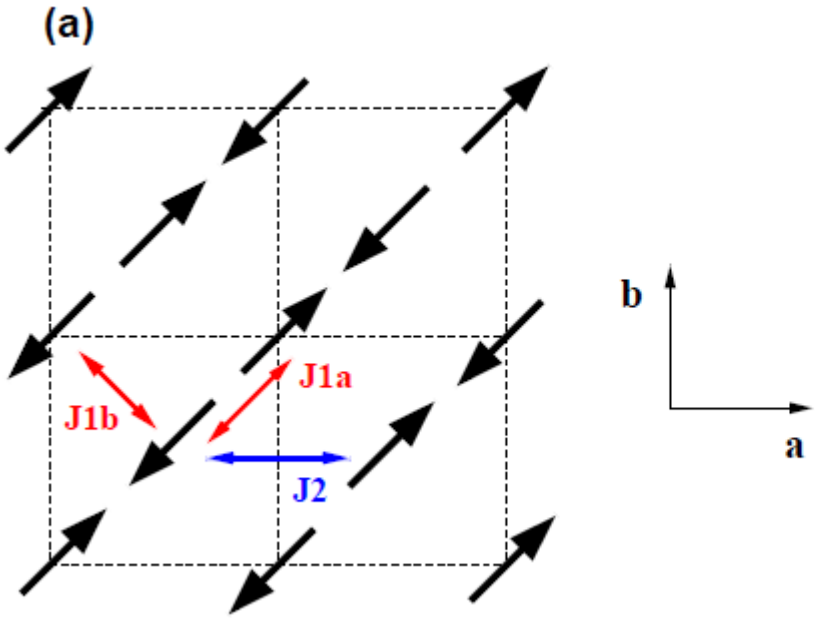
Nesting reduced via doping, pressurization

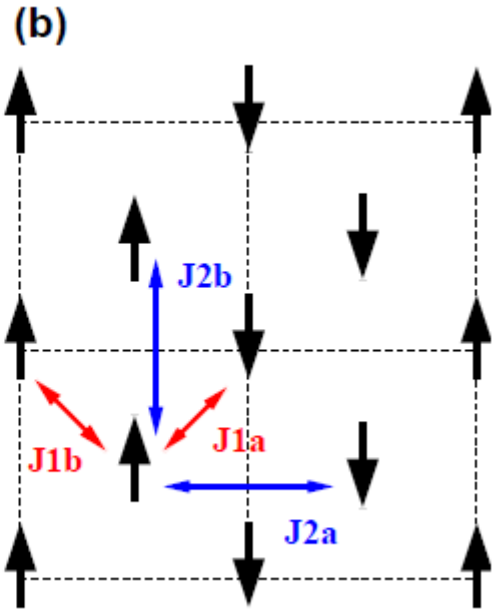
Suppression of phase transition key to produce SC

Y Mizuguchi *et al.*, Appl. Phys. Lett. **94**, 012503 (2009)

$Fe_{1+x}Te$

<FeAs SCs>





<$Fe_{1+x}Te$>

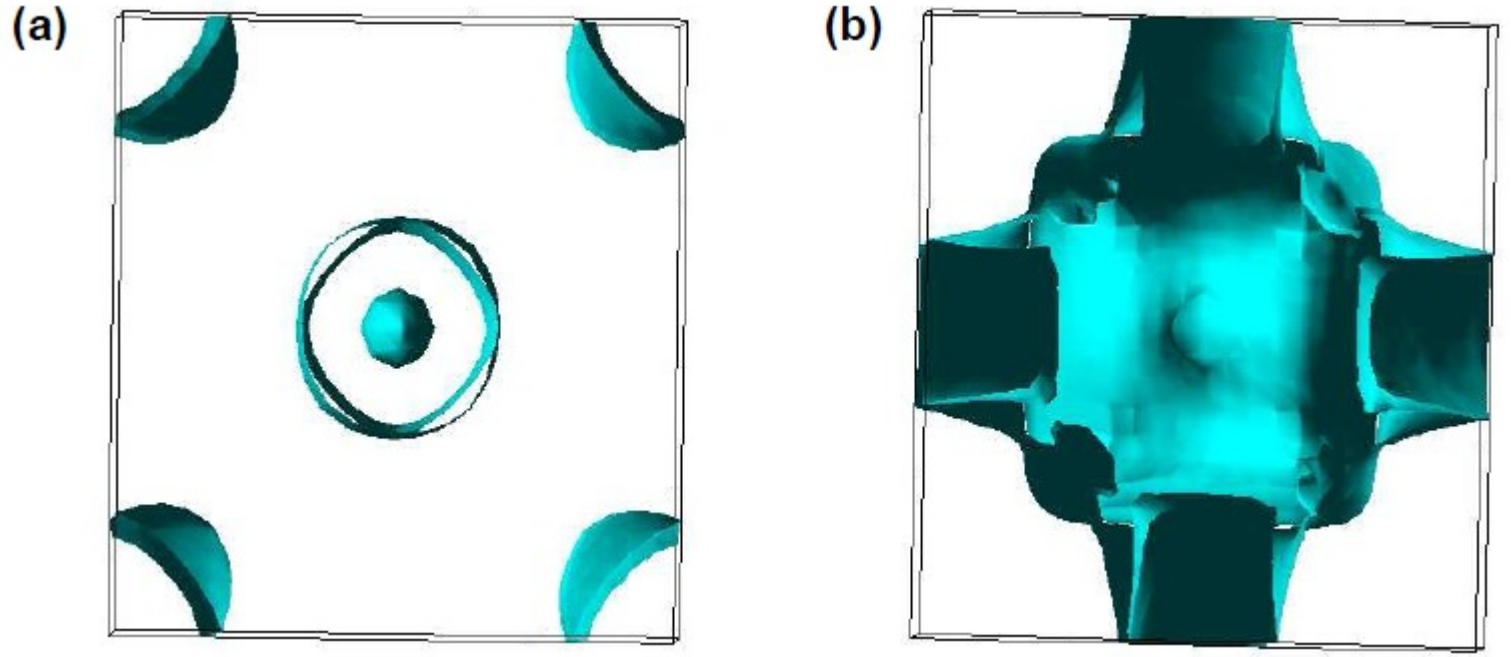
Neutron scattering reveals double-strip AFM ordering

Fe-doped calculations support this ordering

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

Spin ordering becomes incommensurate at x ~ 0.141

S. Li *et al.,* Phys. Rev. B **79**, 054503 (2009)
M. J. Han and S. Y. Savrasov, arXiv:0903.2896v2 (2009)



<FeTe>

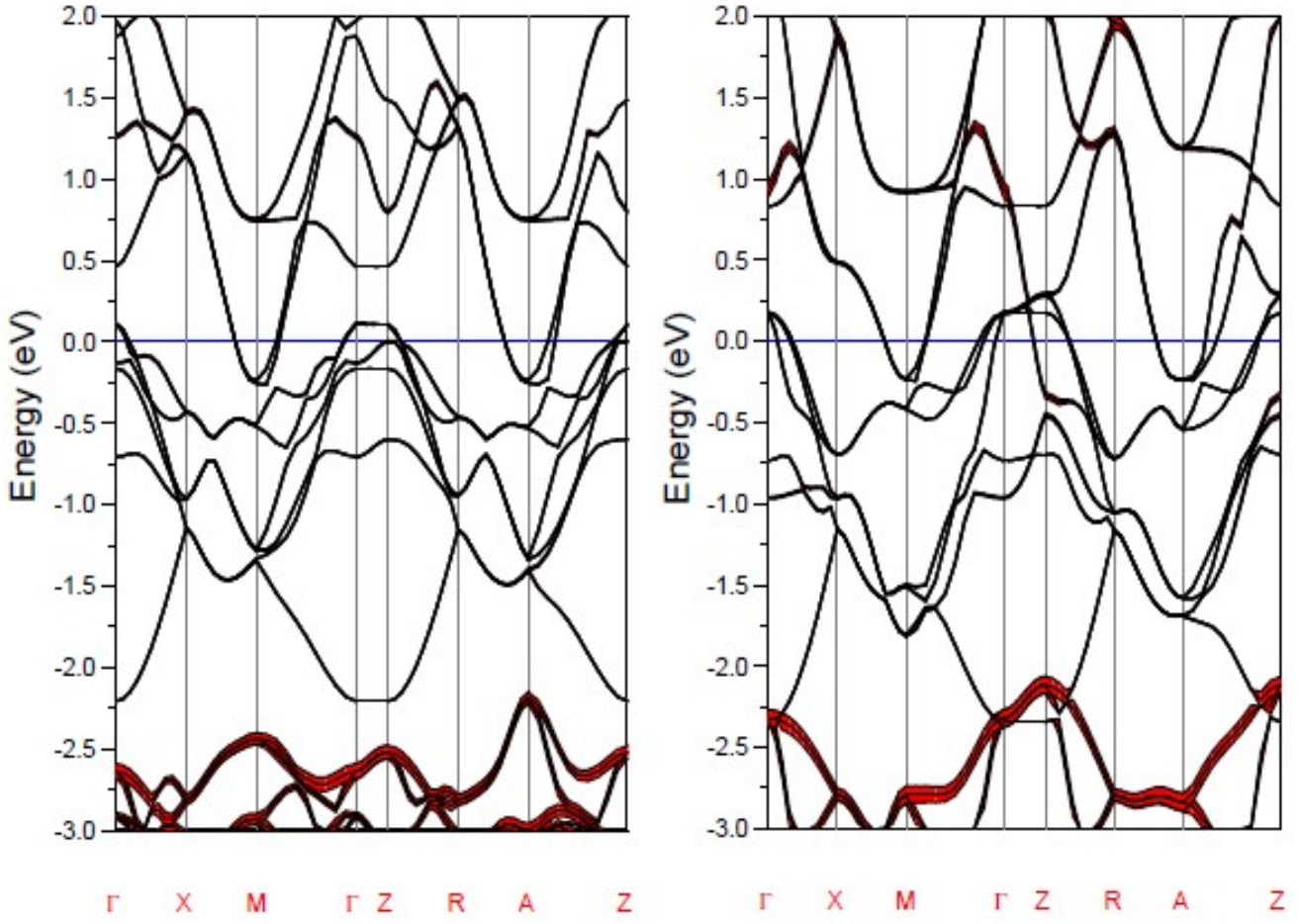
<$Fe_{1+x}Te$>

(π, 0) nesting appears upon doping

(π, π) nesting suppressed

M. J. Han and S. Y. Savrasov, arXiv:0903.2896v2 (2009)

<LaFeAsO>



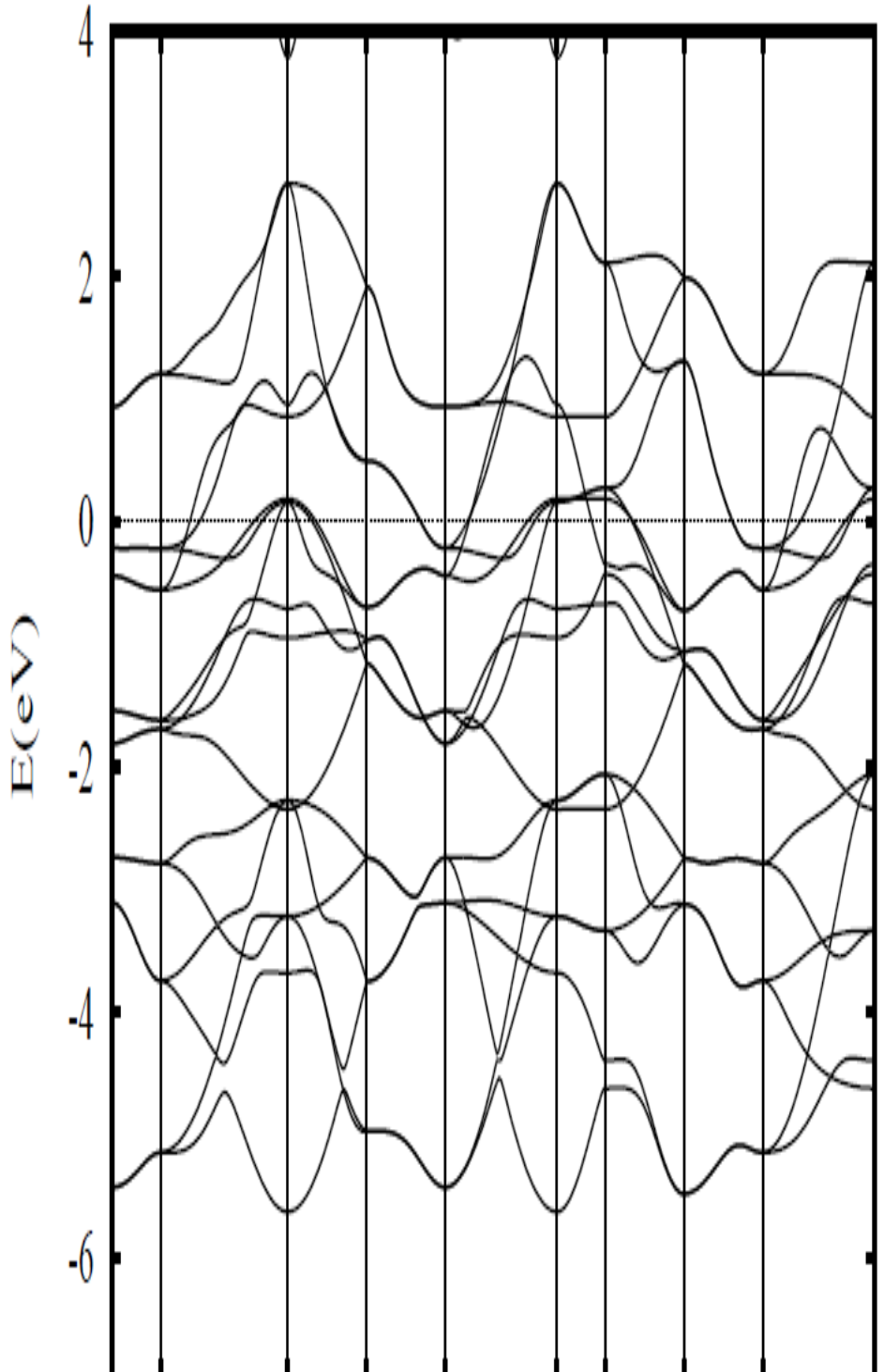
<FeTe>

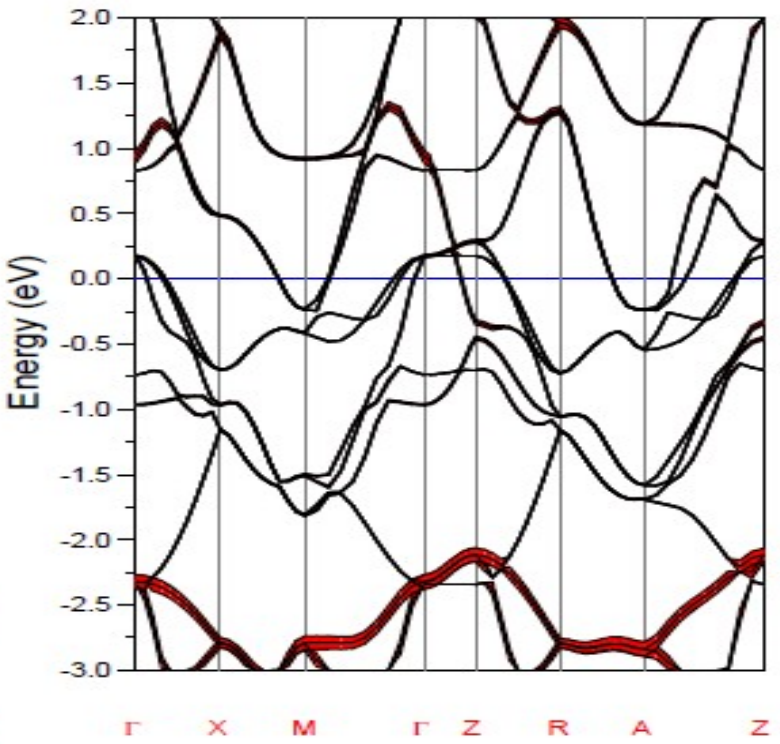
Te *p*-bands hybridize with Fe *d*-bands

Band crossing observed near Fermi level

No band crossing across X

M. J. Han and S. Y. Savrasov, arXiv:0903.2896v2 (2009)


E(eV)
4
2
0
-2
-4
-6


Energy (eV)
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
-1.5
-2.0
-2.5
-3.0
Γ X M Γ Z R A Z

Summary

- 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