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Superconductivity in Fe-based ladder compound $BaFe_2S_3$

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Outline

- Introduction
- Fe-based ladder material $BaFe_2S_3$
  - ✓ Basic physical properties
  - ✓ High-pressure effect
  - ✓ Substitution effect
- Other possible parent materials $BaFe_2Se_3$, $CsFe_2Se_3$
- Summary

Collaborators

Synthesis and Characterization: Y. Hirata, F. Du, Y. Ueda (ISSP)

High-pressure (DAC): H. Takahashi (Nihon Univ.)

High-pressure (Cubic): Y. Uwatoko, T. Yamauchi (ISSP)

Neutron: T.J. Sato, Y. Nambu (Tohoku Univ.), M. Avdeev (ANSTO)

Mossbauer: T. Kawakami (Nihon Univ.)

NMR: M. Ito (Nagoya Univ.)

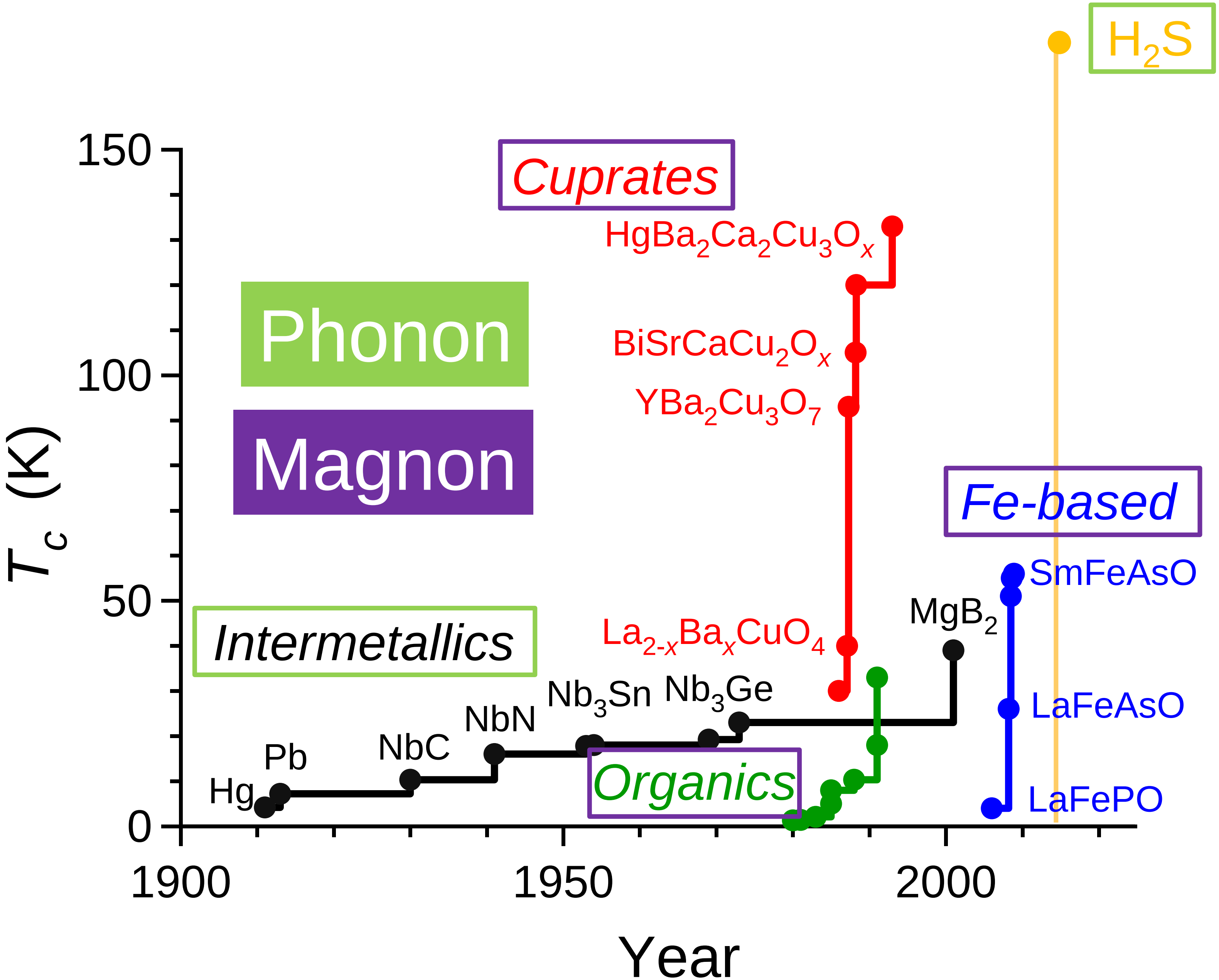
PES: T. Mizokawa (Waseda Univ.)

XRD: J. Yamaura (Tokyo Tech.)

Optics: H. Okamura (Tokushima Univ.)

Theory: R. Arita (Riken)

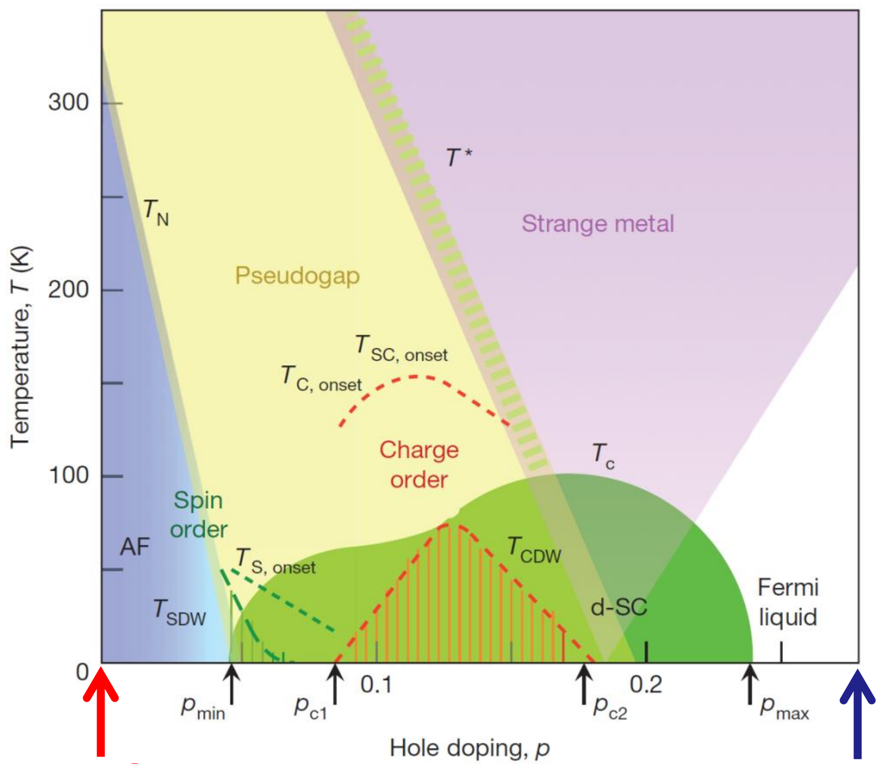
Superconducting transition temperature



Cuprates and organics superconductors

Cuprates

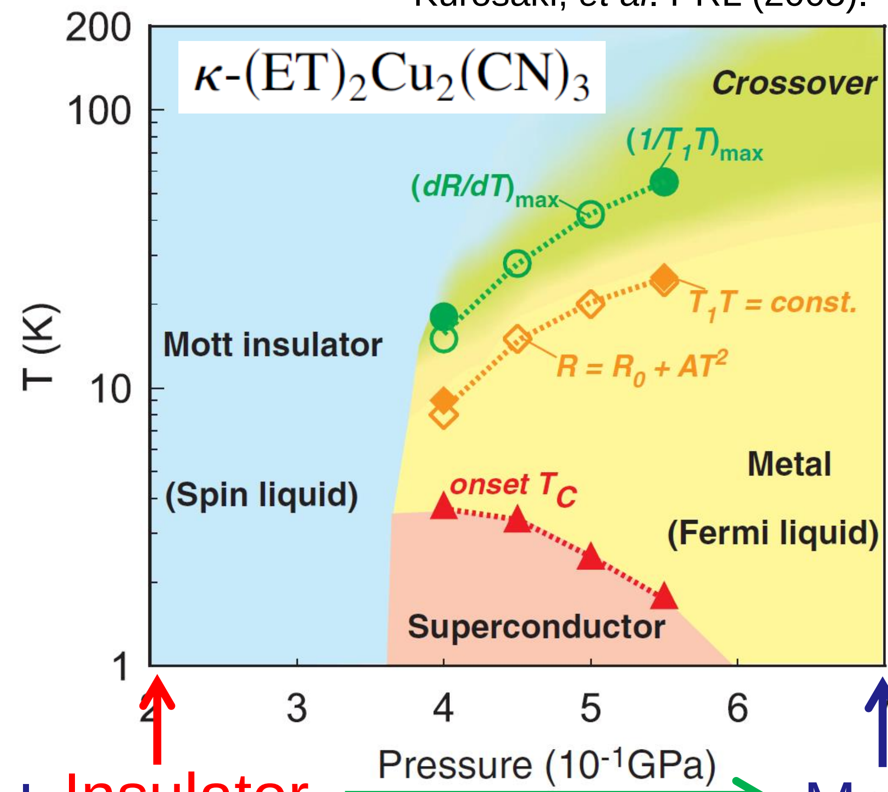
Keimer, *et al*. Nature (2015).



Insulator → Filling → Metal

Organics

Kurosaki, *et al*. PRL (2005).

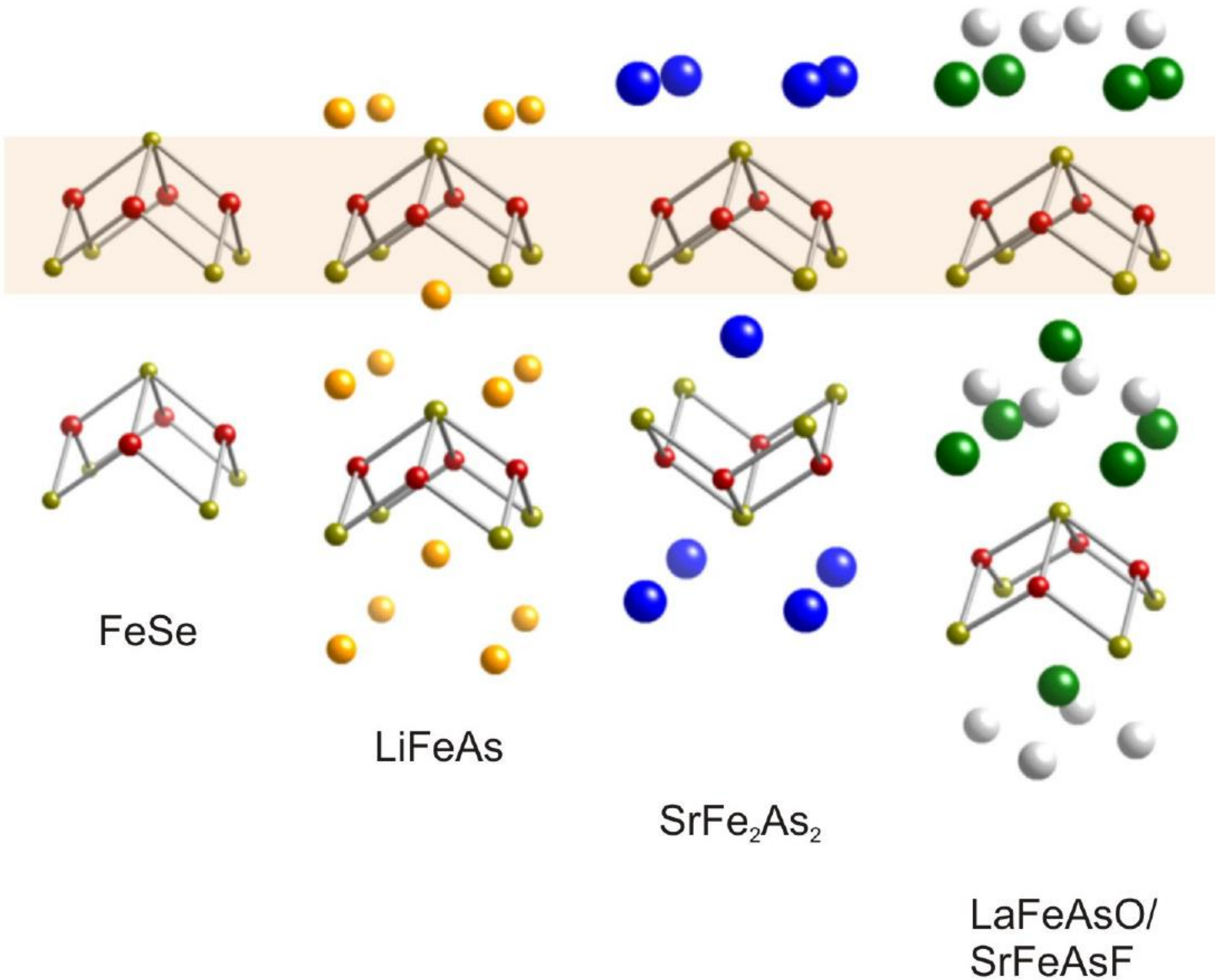


Insulator → Bandwidth → Metal

- SC appears in the vicinity of Mott transition.
- Strong electron correlation effect. $U \sim 1$eV.

Fe-based superconductors

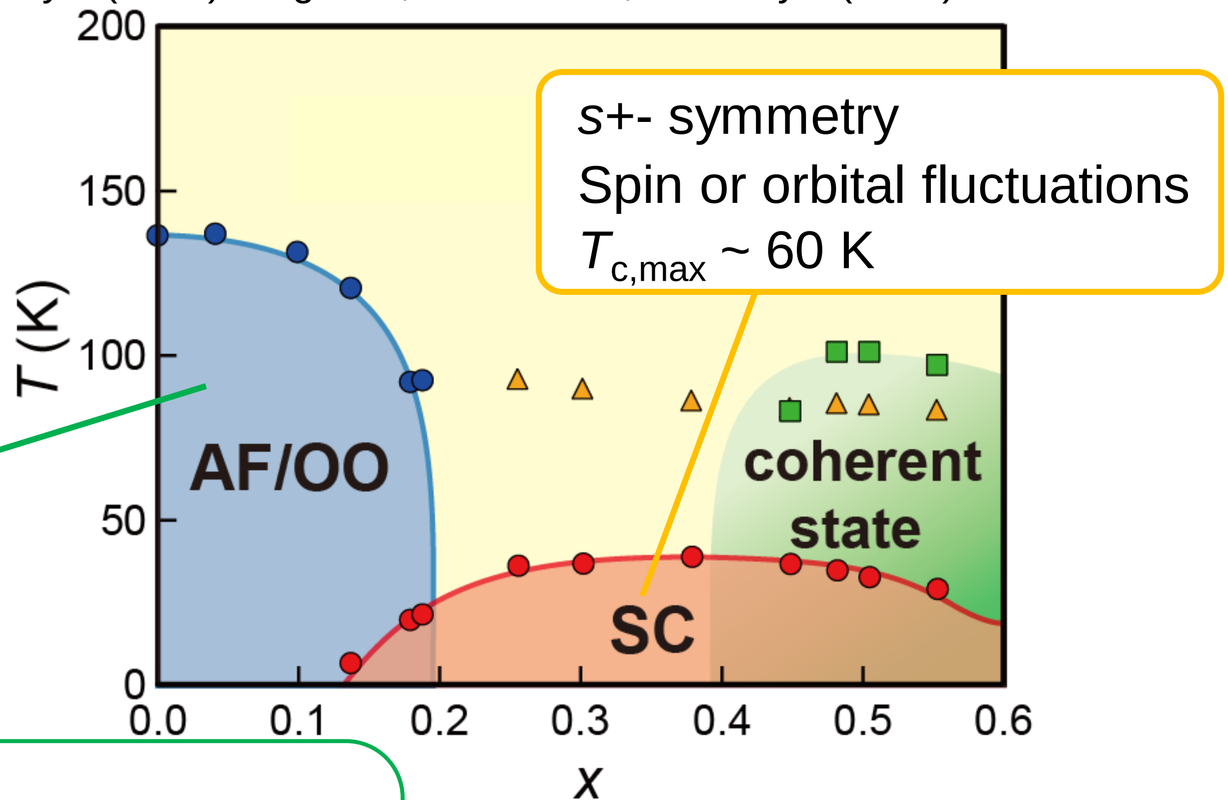
Hosono, JACS (2008), Paglione,and Greene, Nat. Phys. (2010).

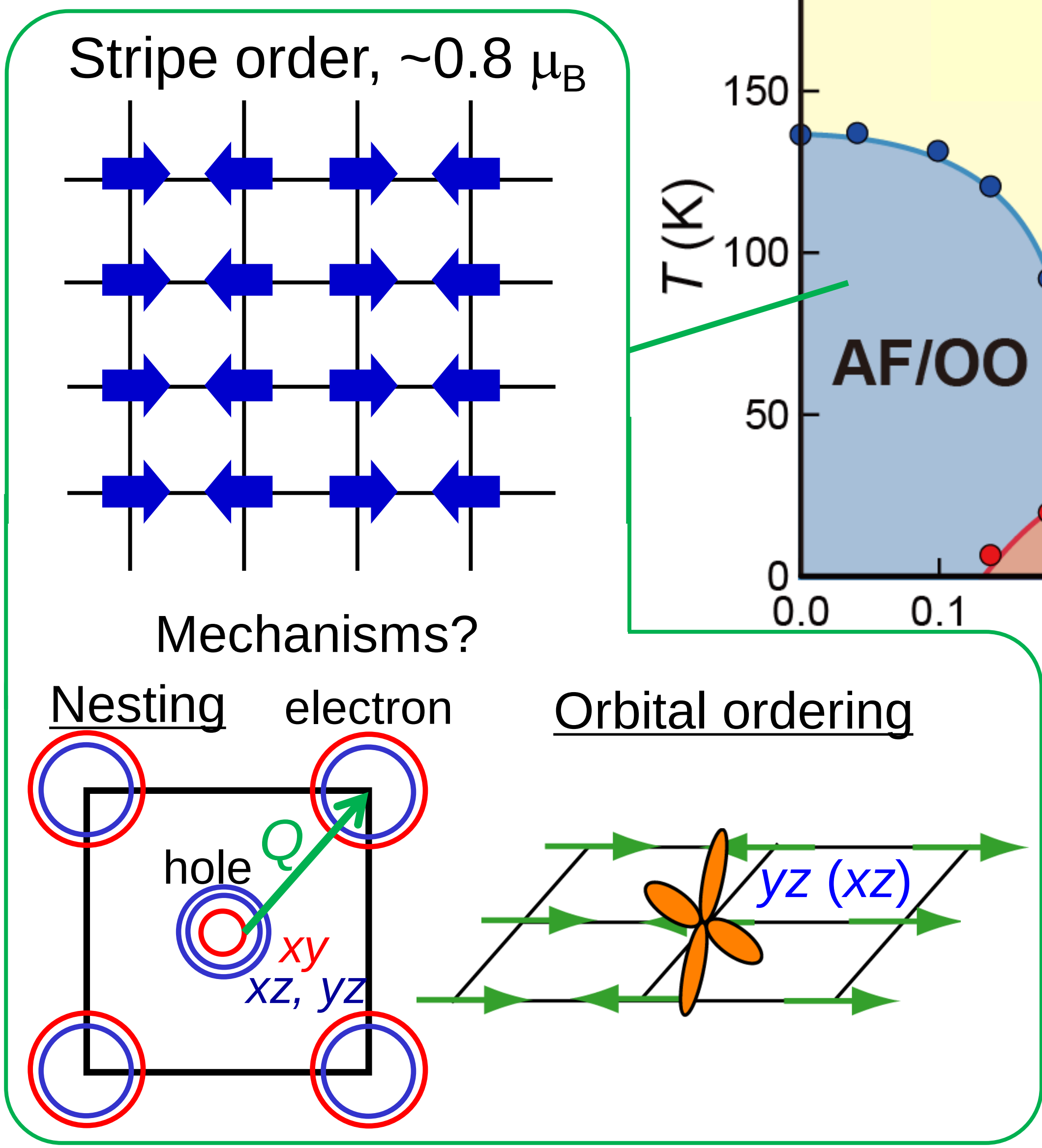


- Square lattice of Fe atoms.
- Fe^{2+} coordinated by As or Se tetrahedrally.

Fe-based superconductors

Dai, Hu, Dagotto, Nat. Phys. (2012). Paglione, and Greene, Nat. Phys. (2010).





Pressure

Chemical substitution

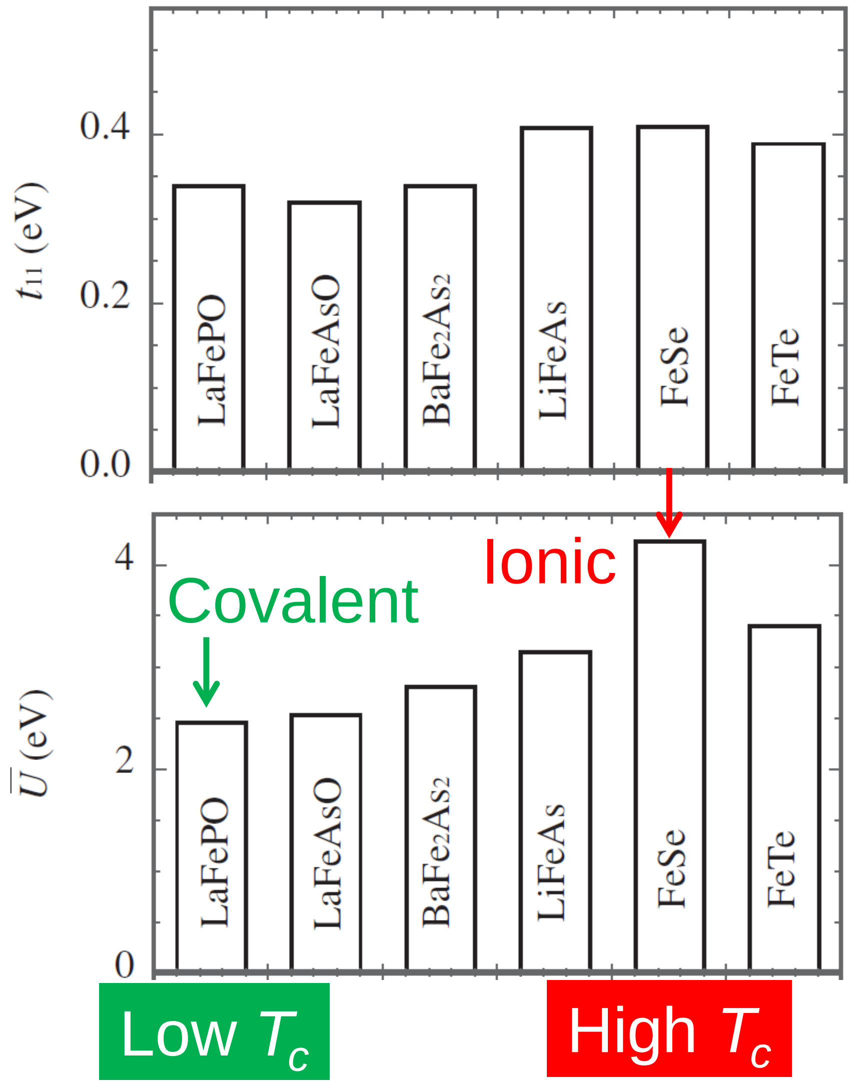
$Ba_{1-x}K_xFe_2As_2$

$BaFe_{2-y}Co_yAs_2$

- All phases are <u>metal</u>.

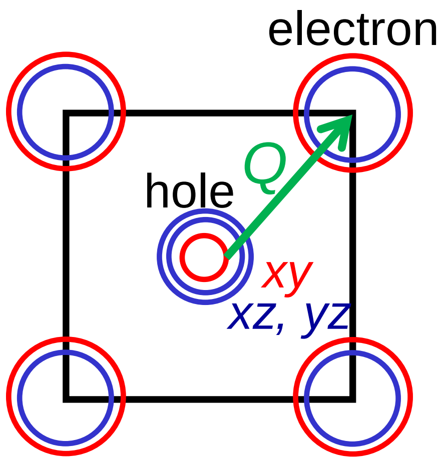
Electron correlation in Fe-based SCs

Material dependence



T. Miyake, *et al*., JPSJ **79**, 044705 (2010).

Orbital dependence



Renormalization factor *z*

	LaFeAsO	FeSe
z^2	0.61	0.38
x^2-y^2	0.66	0.47
xy	0.61	0.20
yz/zx	0.60	0.28

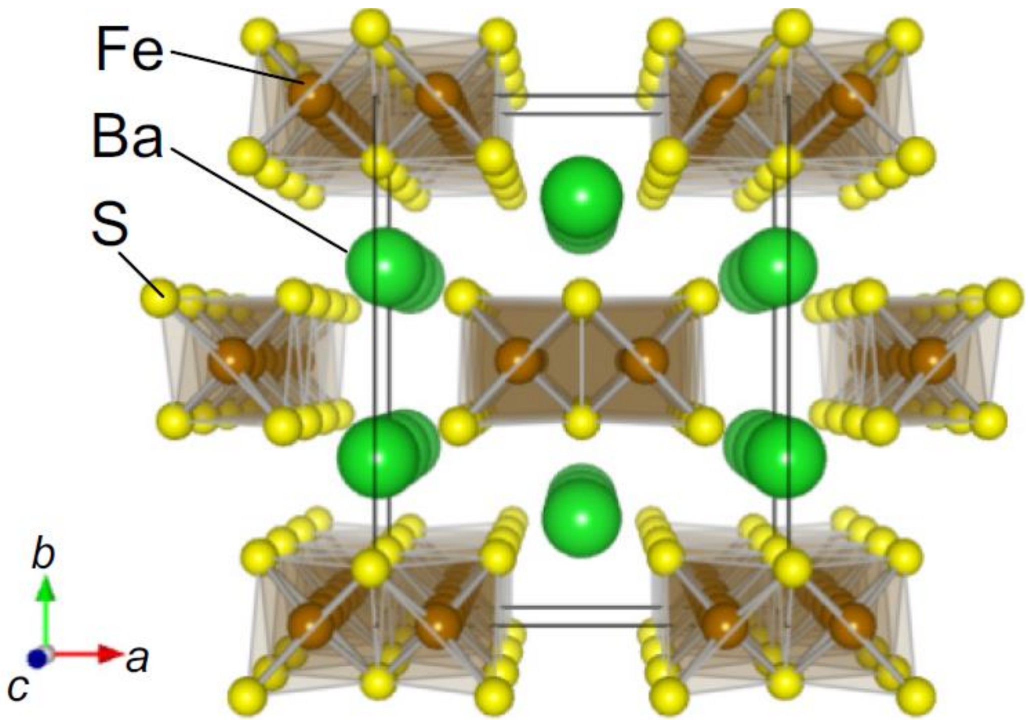
M. Aichhorn, *et al*., PRB **80**, 085101 (2009).
PRB **82**, 064504 (2010).

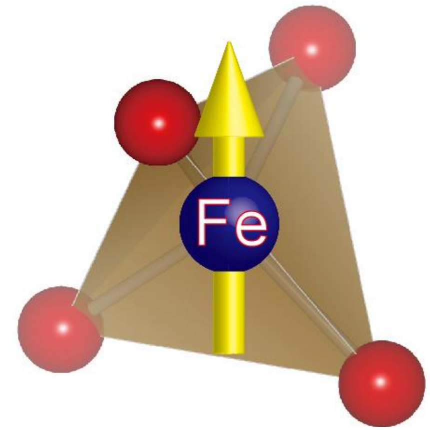
Fe-based ladder compound $BaFe_2S_3$

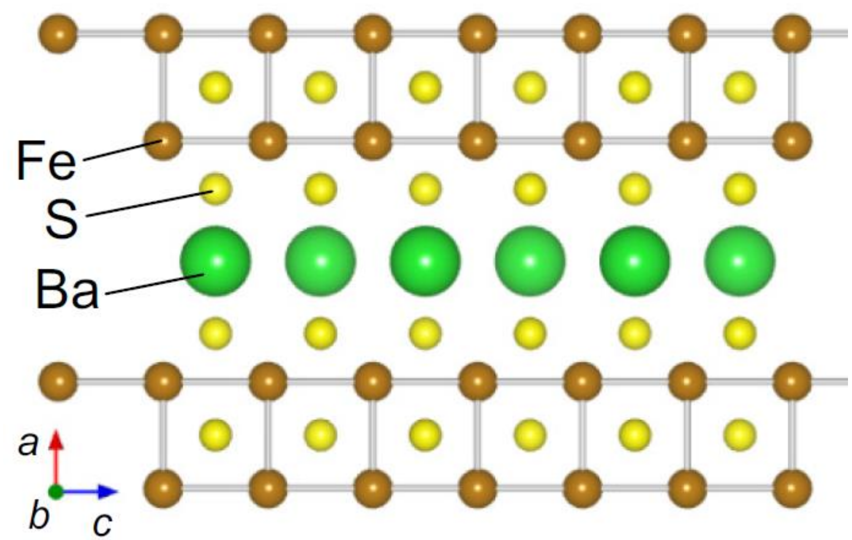
What happens if we lower the dimensionality and reduce the bandwidth? We can see the strong correlation effect.

$BaFe_2S_3$

Fe^{2+}: $(3d)^6$





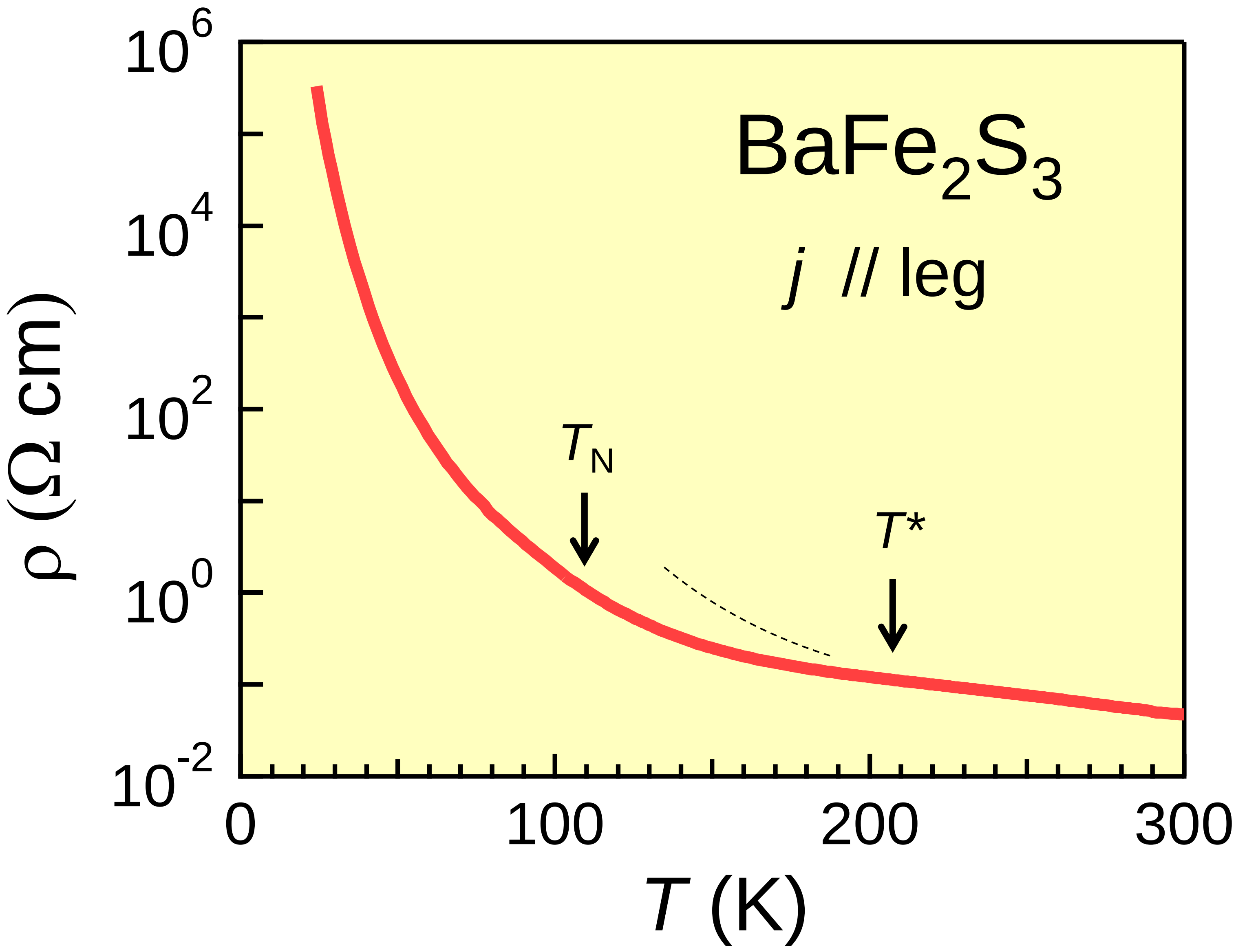


Orthorhombic, *Cmcm*

Earlier works: McQueen, Petrovic, Sefat, Dagotto…

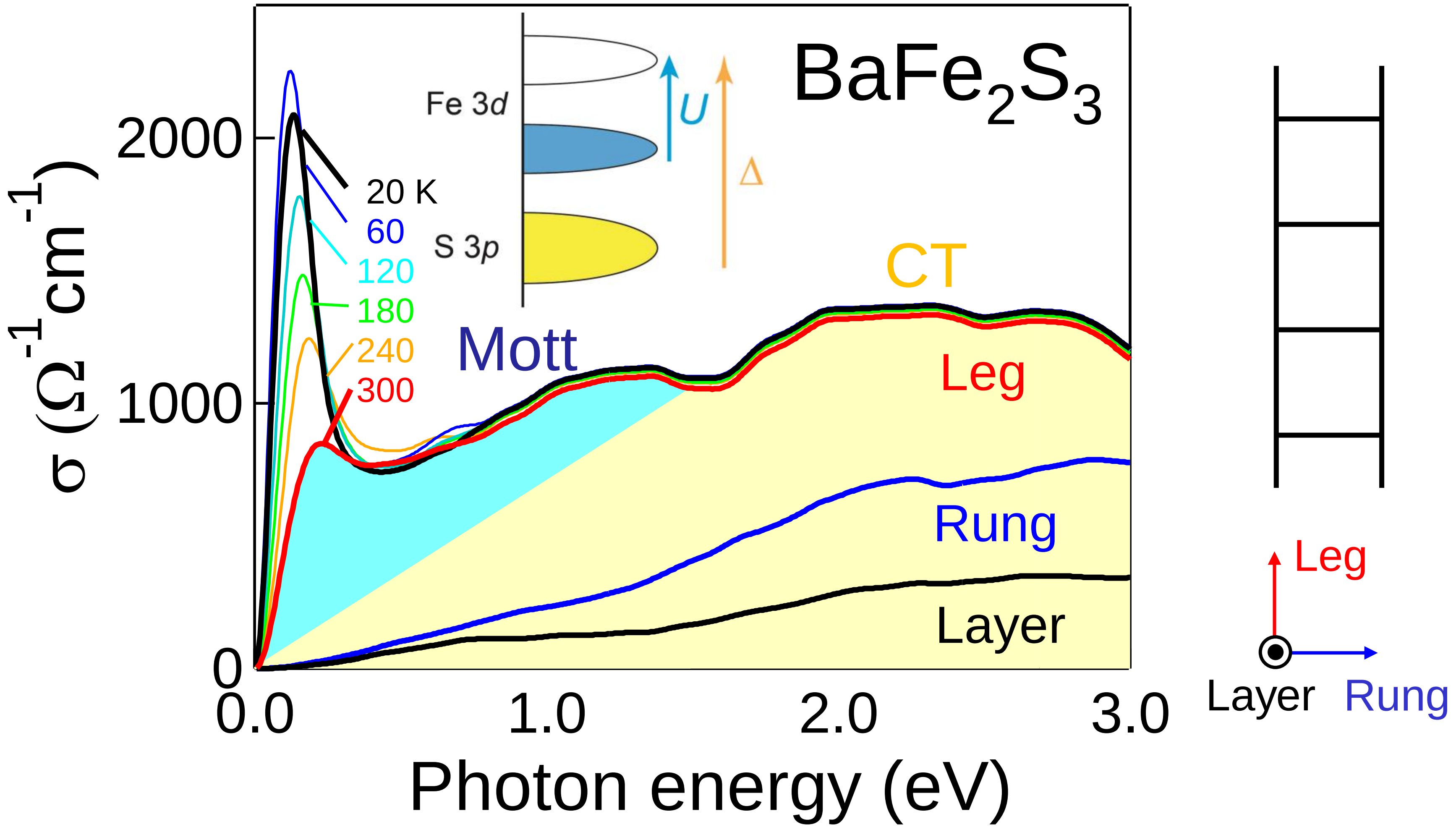
Basic physical properties

Resistivity



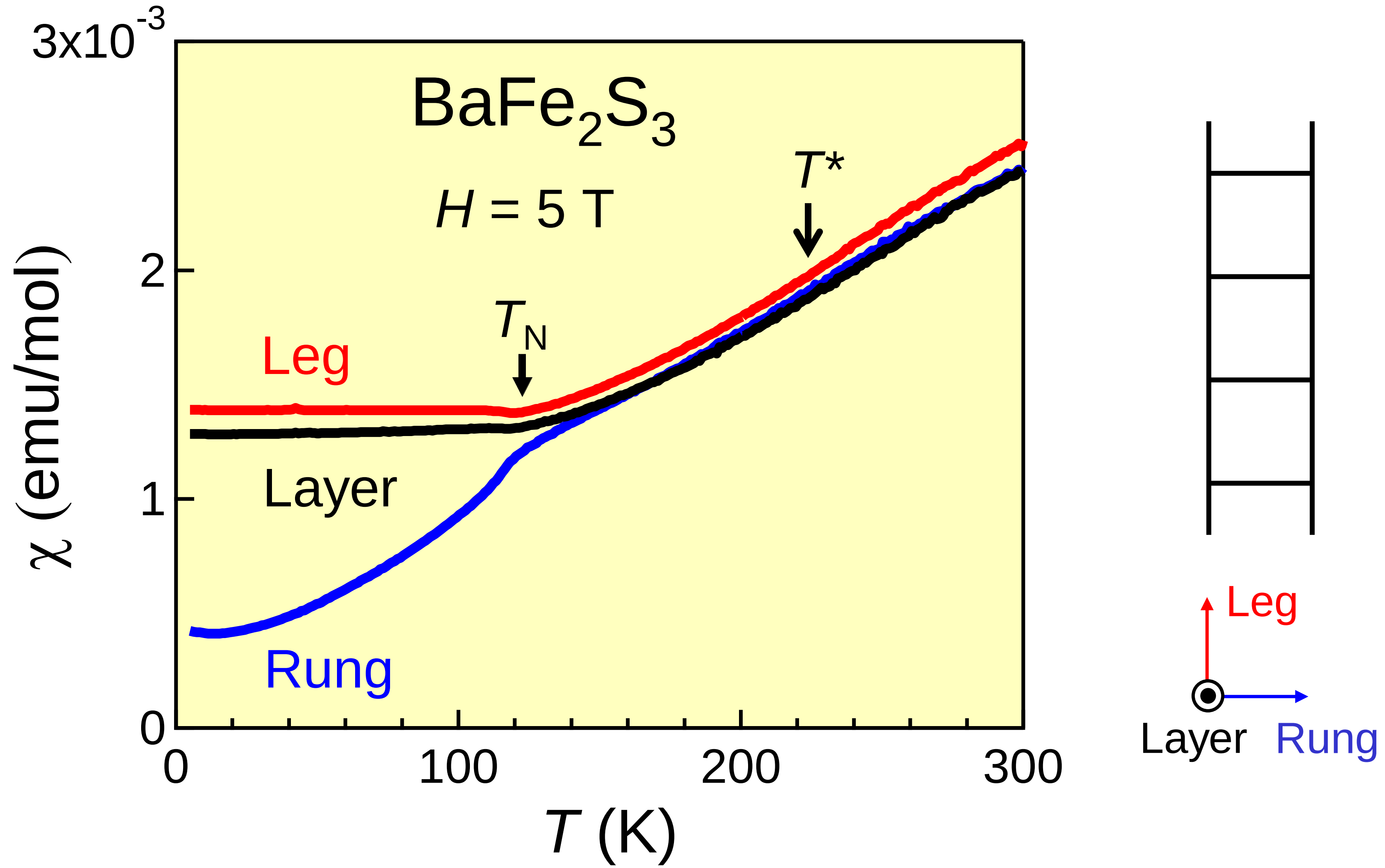
- Mott insulator induced by strong correlation effect.

Optical conductivity



- Quasi-one dimensional electronic state.
- Coherent Fe 3*d* bands below 0.2 eV even in Mott insulator.

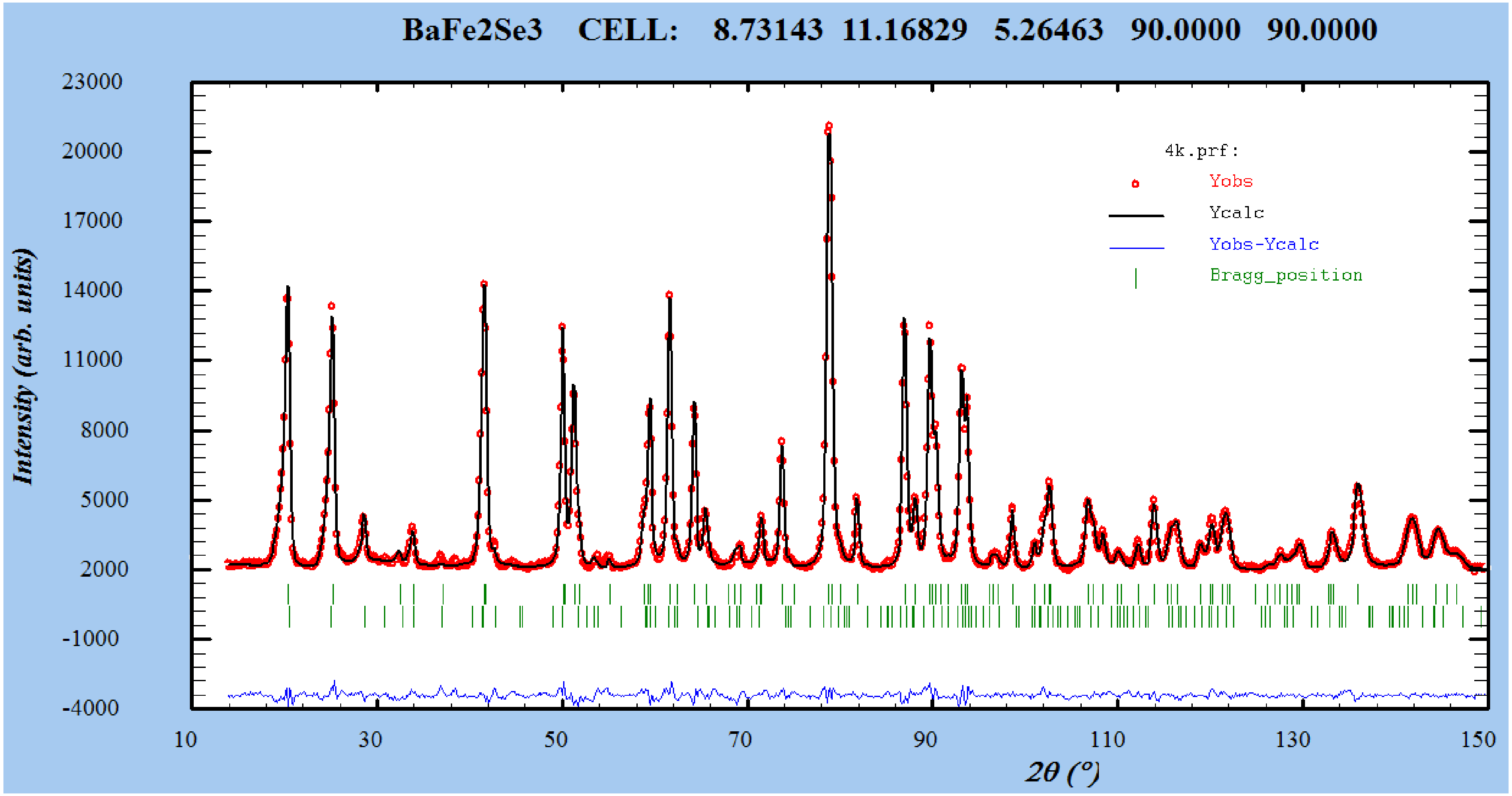
Magnetic susceptibility



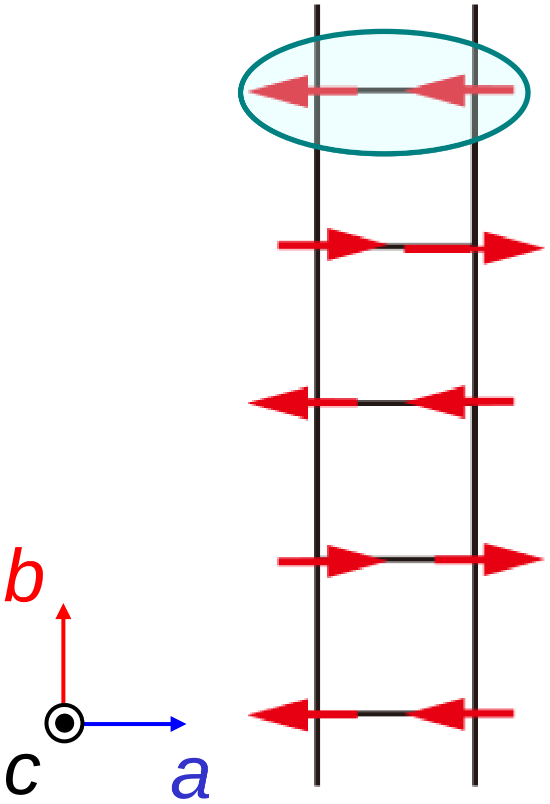
- Decrease in χ on cooling due to quantum fluctuations in 1 D or itinerant nature close to Mott transition.
- Antiferromagnetic order with the rung direction as the easy axis.

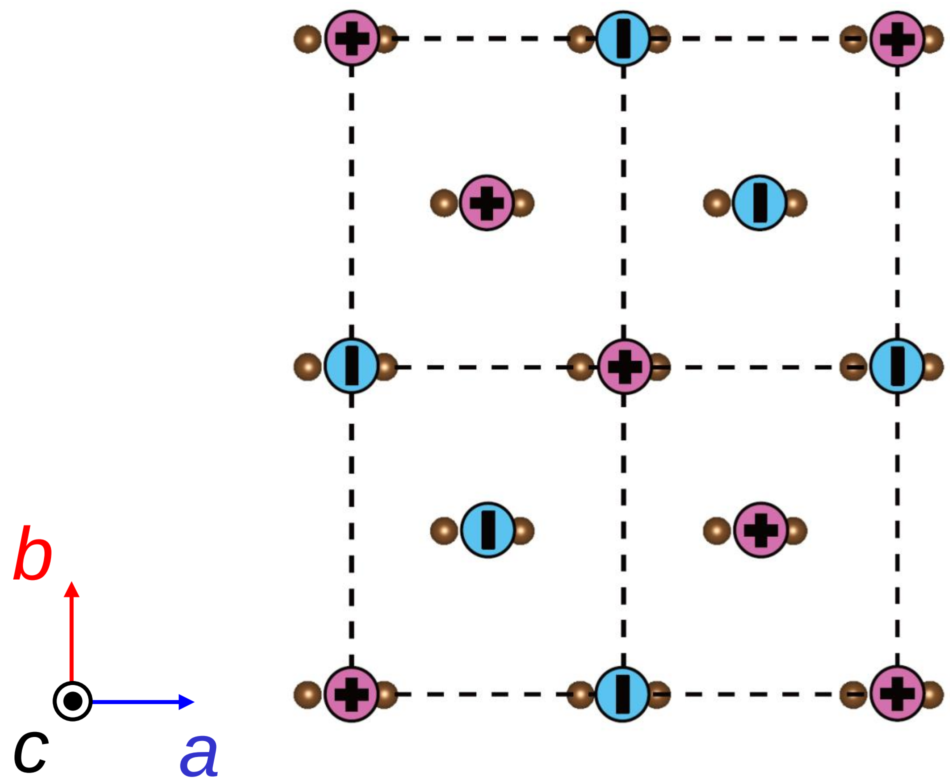
Neutron diffraction

$BaFe_2S_3$



Magnetic structure of $BaFe_2S_3$

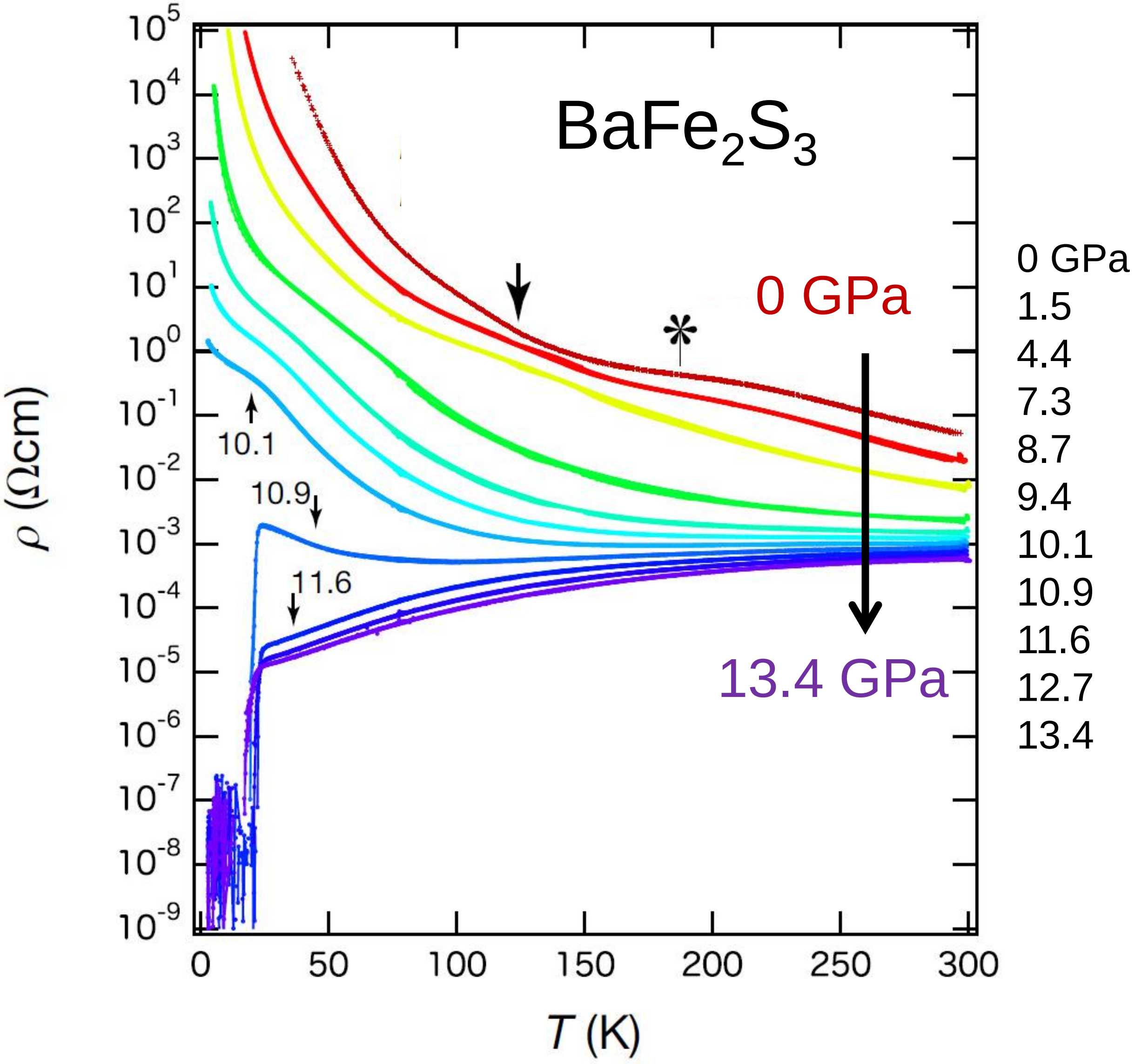




- Stripe-type magnetic ordering.
- Ordered moment is 1.3 μ_B. Much smaller than the high-spin value, 4 μ_B.
- Inter-ladder coupling is ferromagnetic along one direction, and antiferromagnetic to the perpendicular direction.

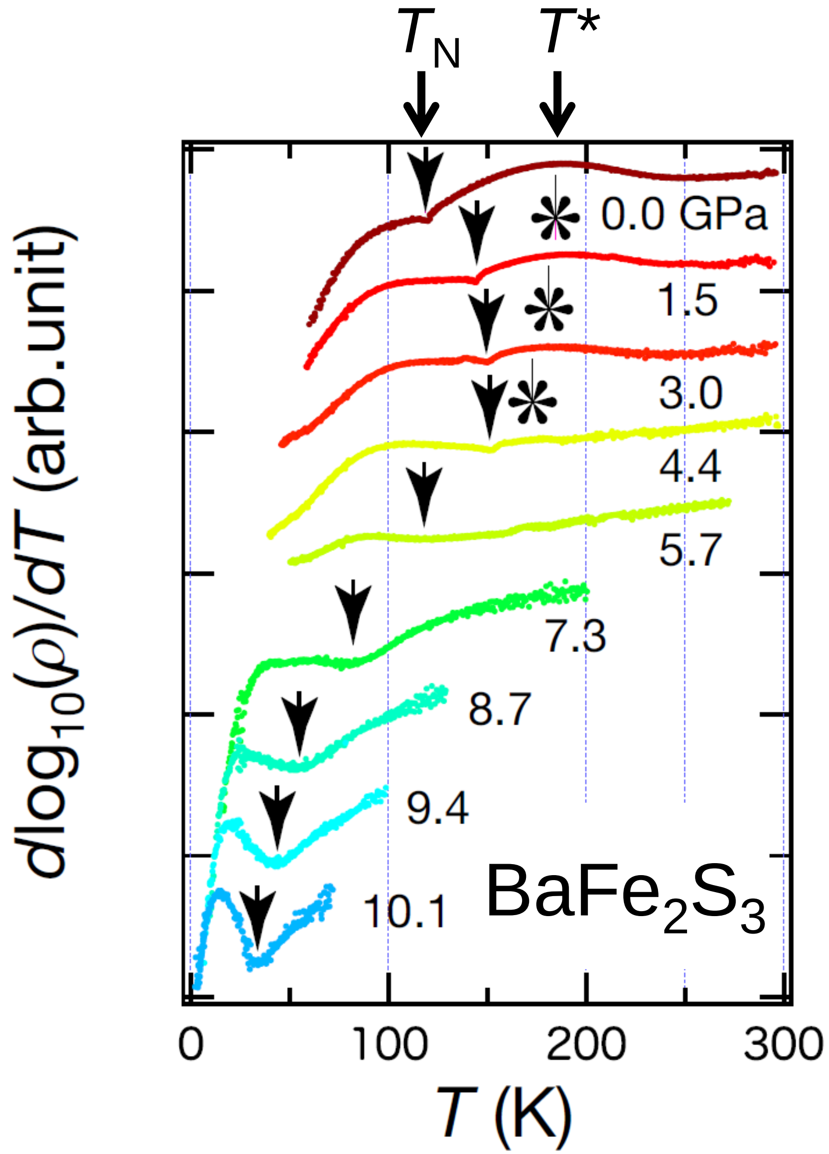
High-pressure effect

$BaFe_2S_3$ under high pressure



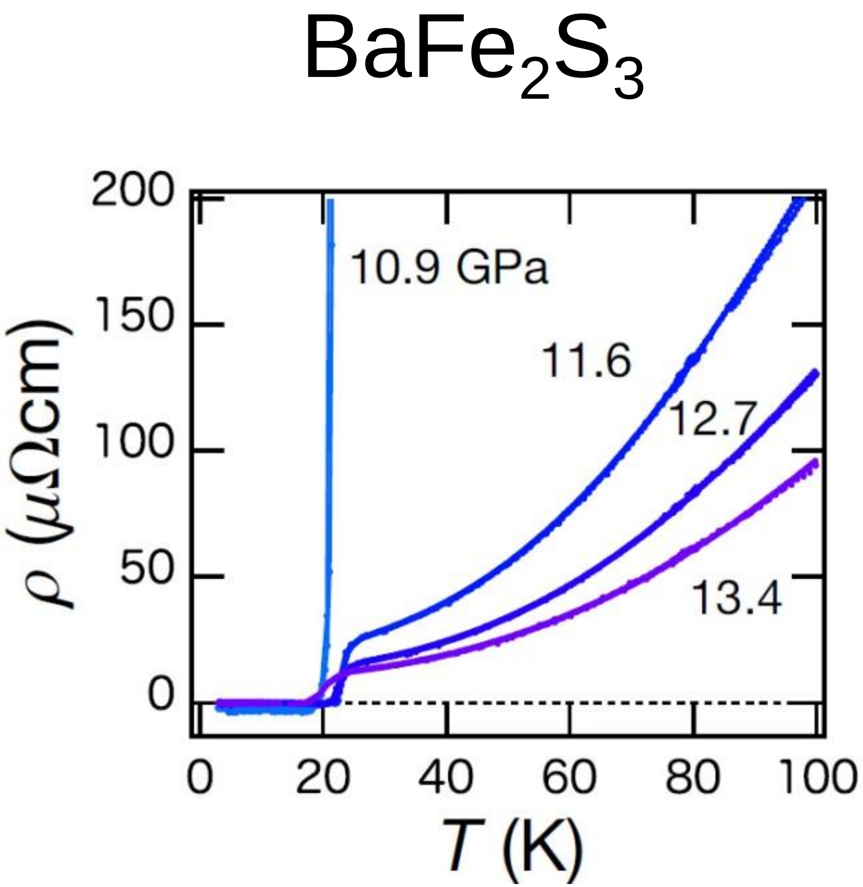
- Bandwidth-control type Mott transition around 11 GPa.
- Superconductivity with T_c = 24 K.

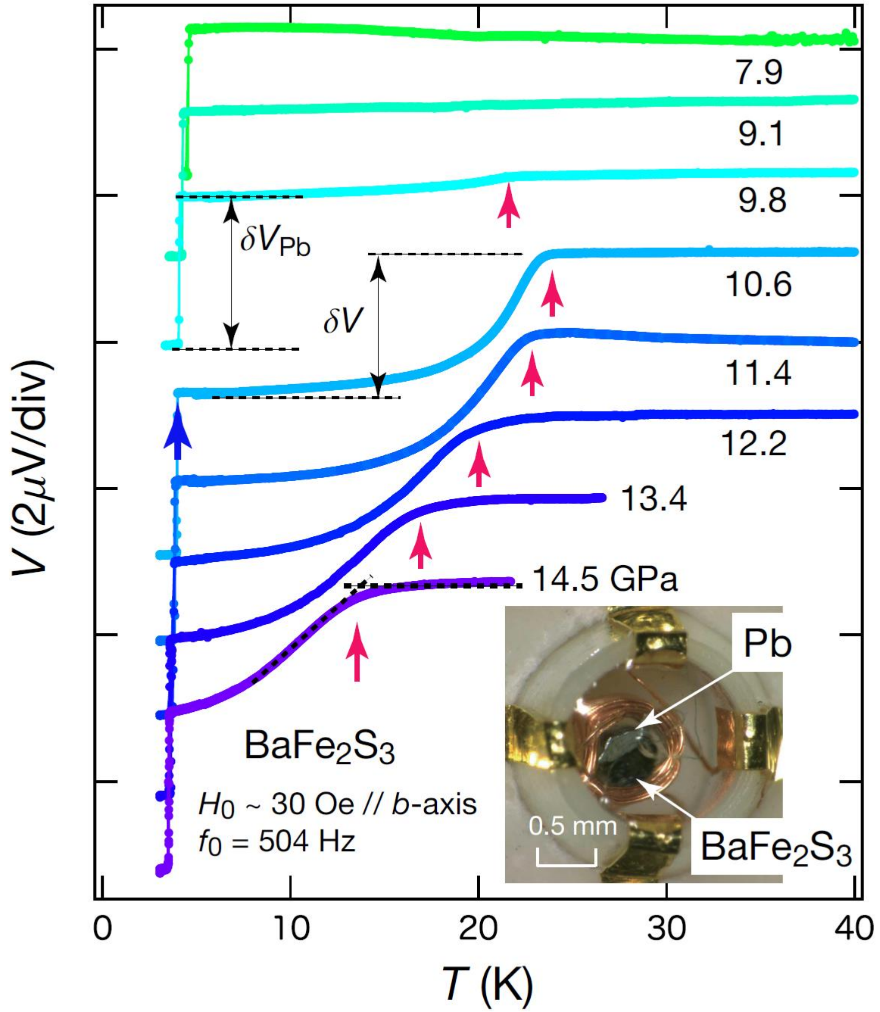
$BaFe_2S_3$ under high pressure



- On applying pressure, T_N increases and merge to T^*at 3 GPa.
- Afterwards, T_N decreases monotonically and vanishes at 11 GPa.

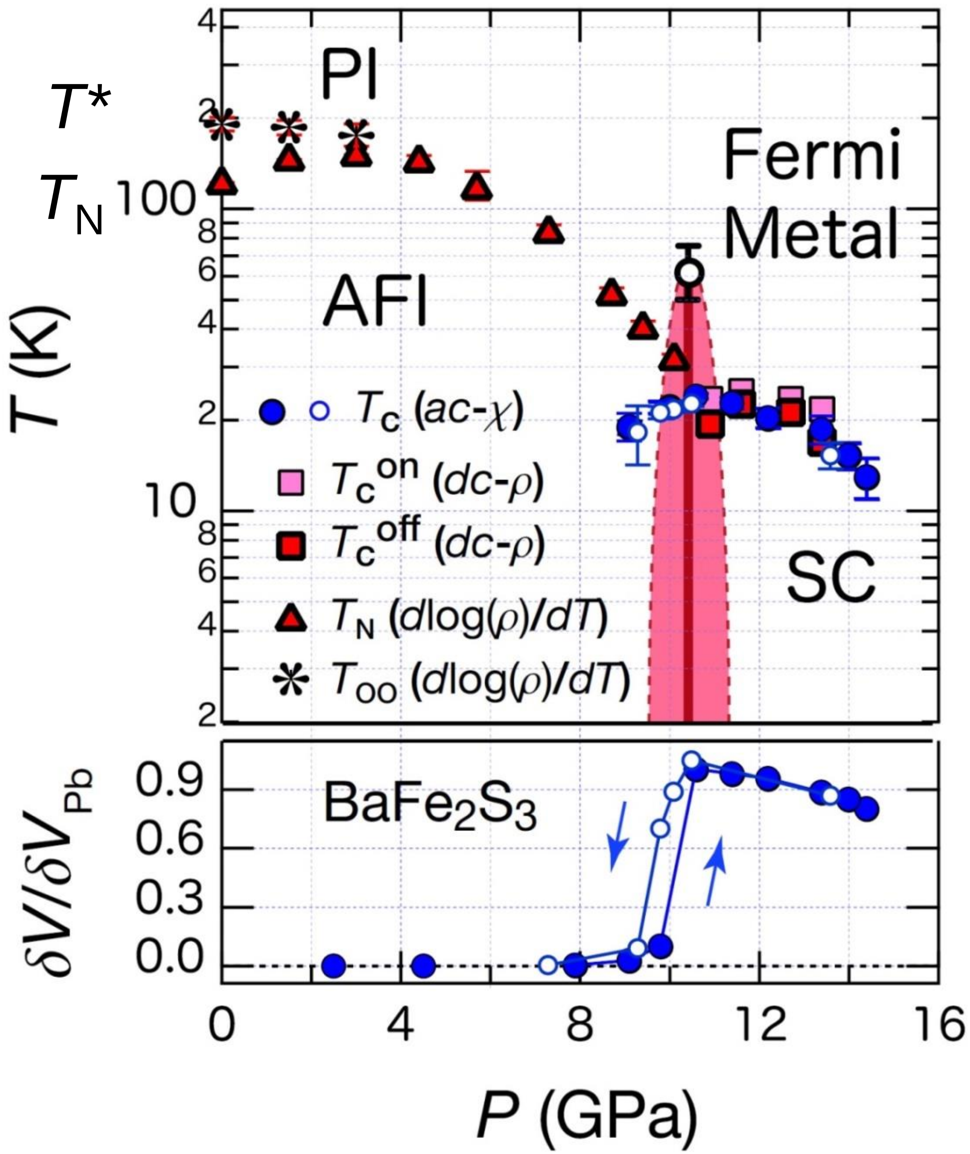
$BaFe_2S_3$ under high pressure





- Fermi liquid behavior $\rho \propto T^2$ above Mott transition.
- Volume fraction, 80 % => Bulkness of superconductivity.

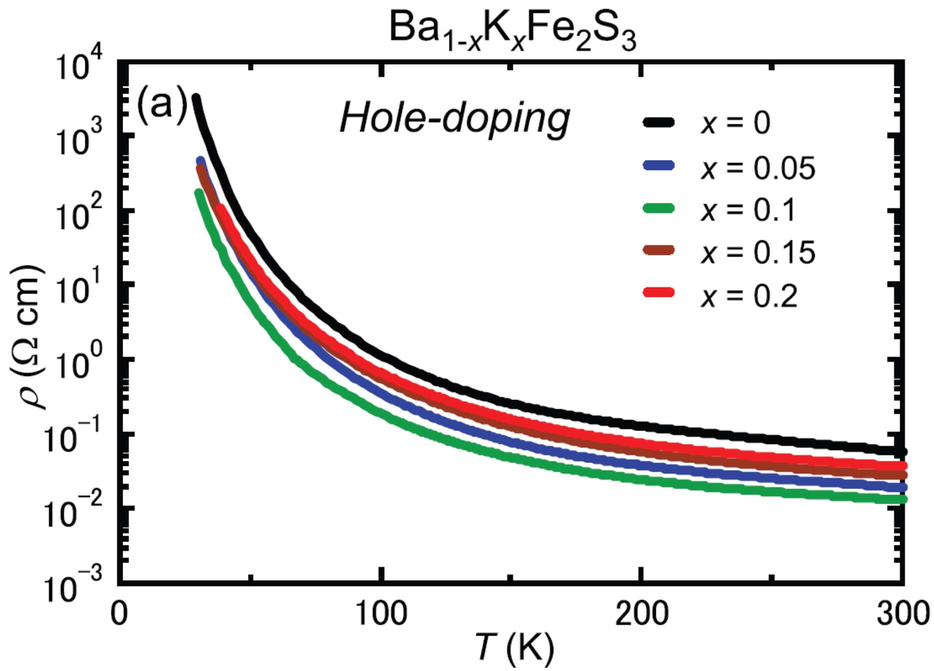
$BaFe_2S_3$ under high pressure

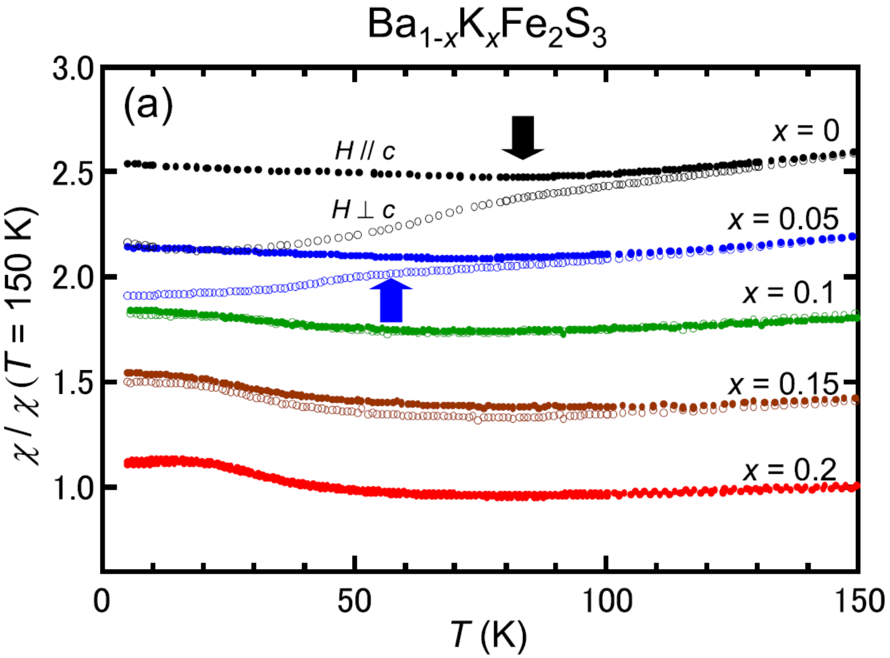


- Similar to the organic superconductors.

Substitution effect

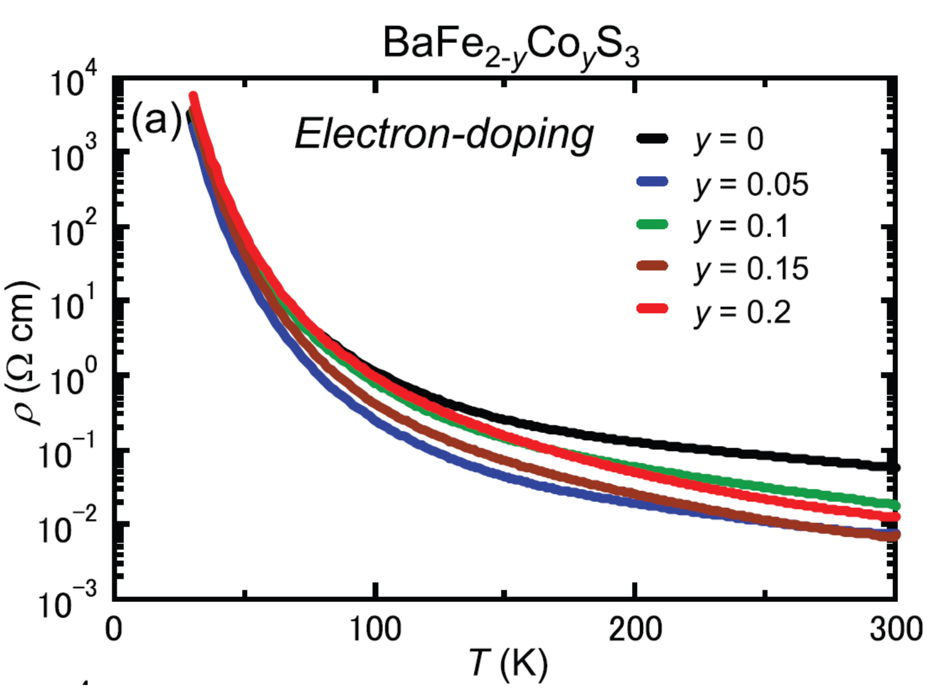
Hole doping: $Ba_{1-x}K_xFe_2S_3$

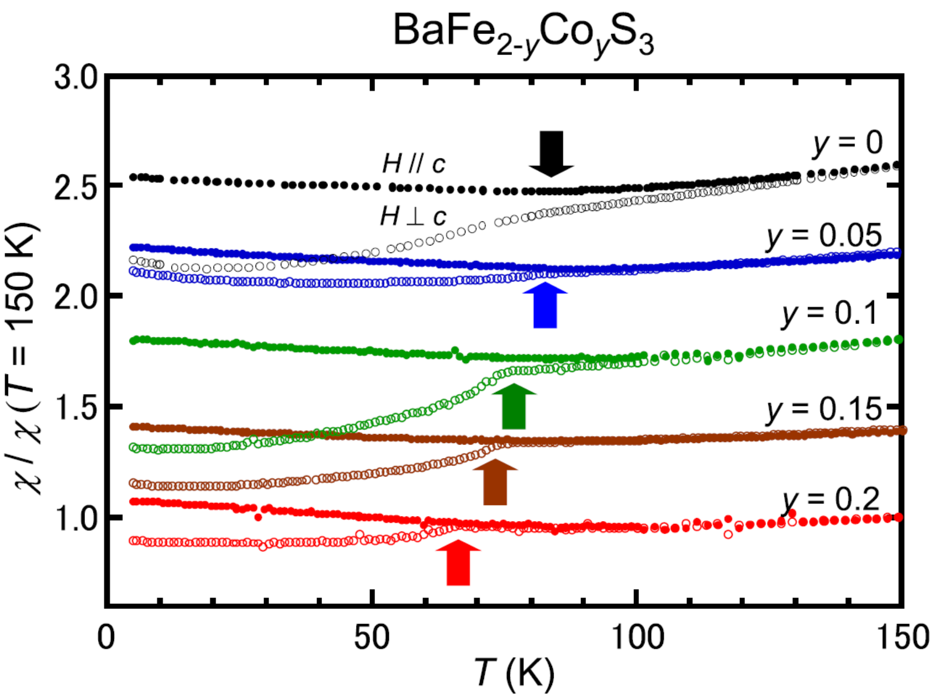




- Robust insulating state.
- Magnetic order is gradually destroyed. However, glassy state is present at large *x* value.

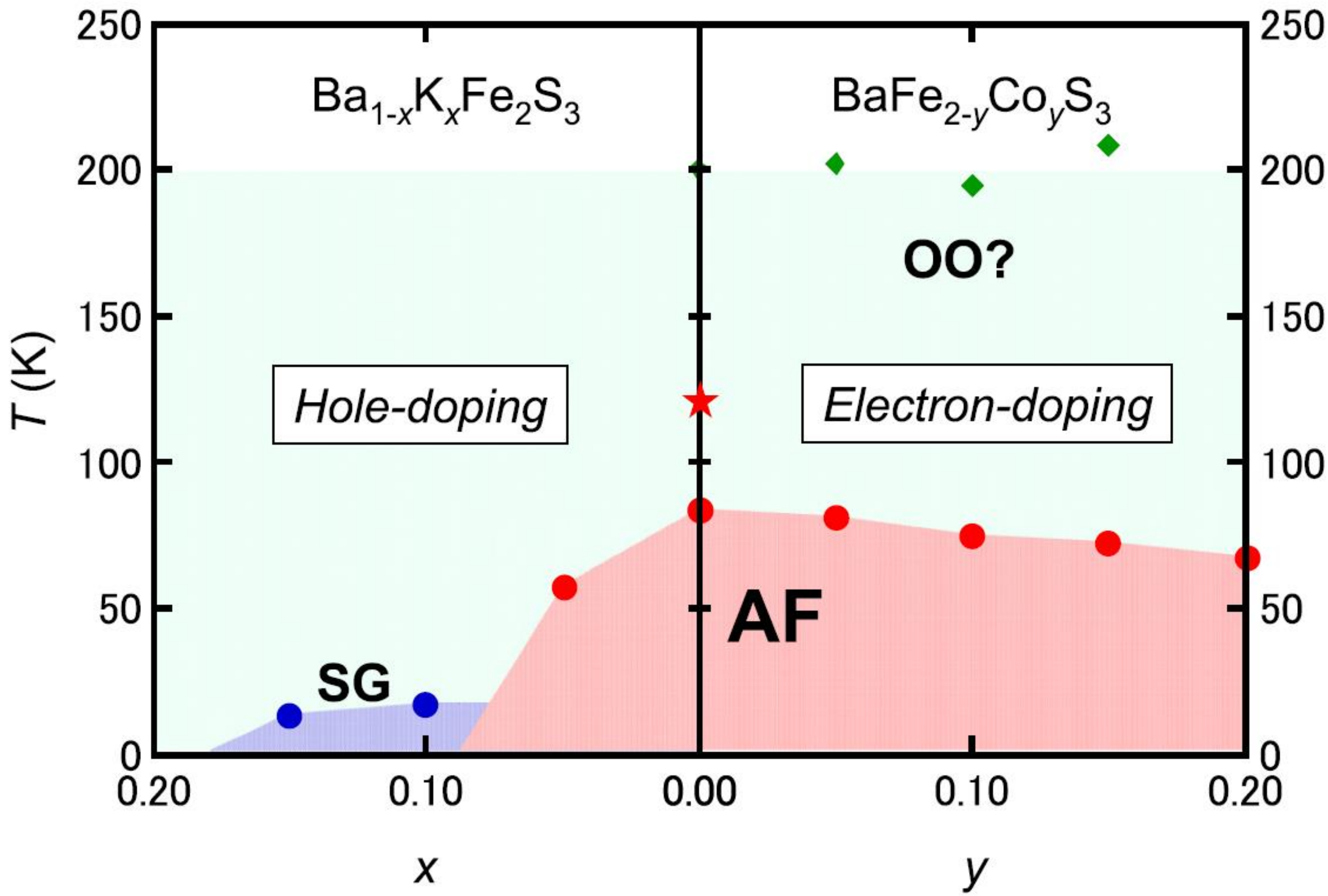
Electron doping: $BaFe_{2-y}Co_yS_3$





- Robust insulating state.
- Magnetic order is also robust.

Phase diagram



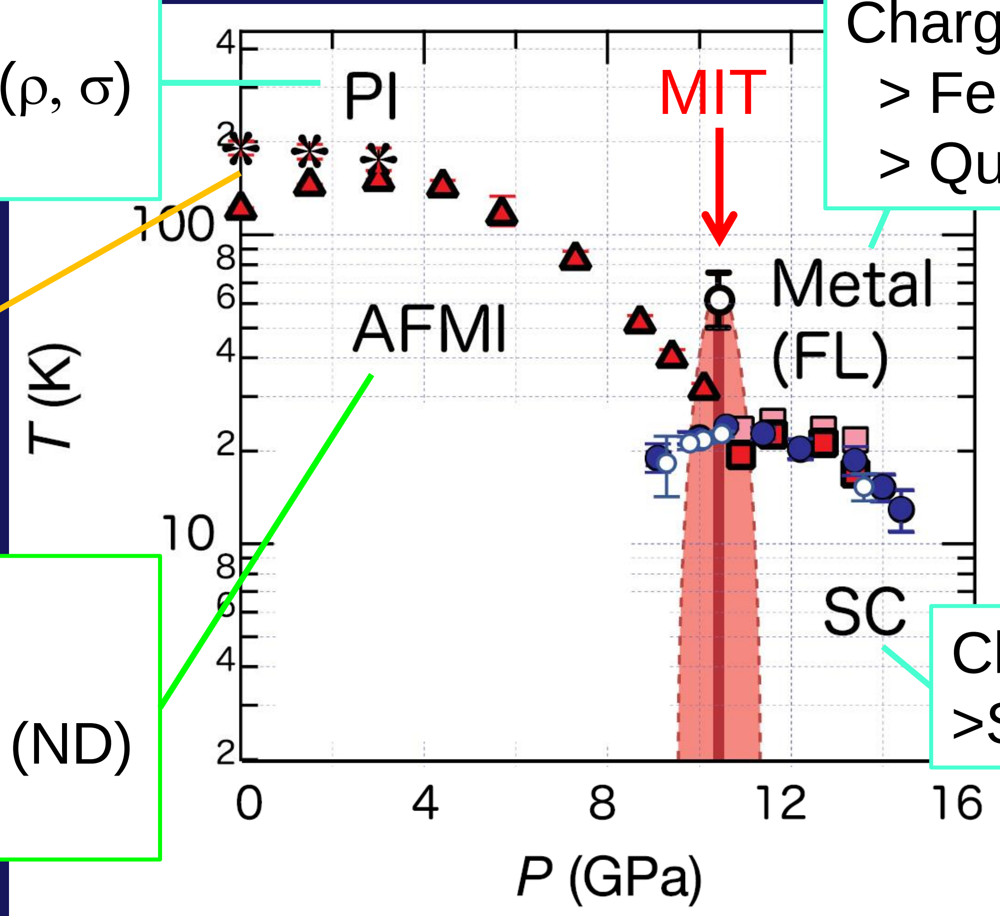
- Electron-hole asymmetry. Opposite to 2 D Fe-based SCs.
- Robust insulating state due to small volume change, ~ 1%.

$BaFe_2S_3$

Charge:
> Localized near MIT(ρ, σ)
> Quasi 1D (σ)

Orbital:
> Ordered? (ρ)

Spin:
> Stripe order (ND)
> Reduced *m*, 1.3 μ_B (ND)
> Quasi 1D (κ)



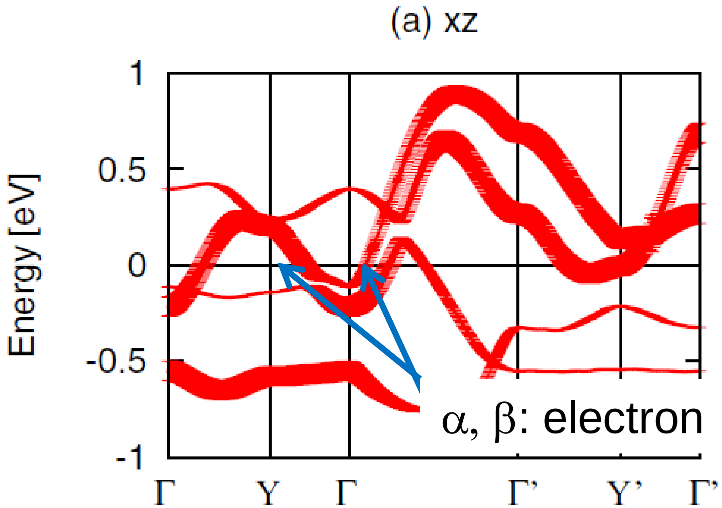
Charge:
> Fermi liquid
> Quasi 2D (σ)

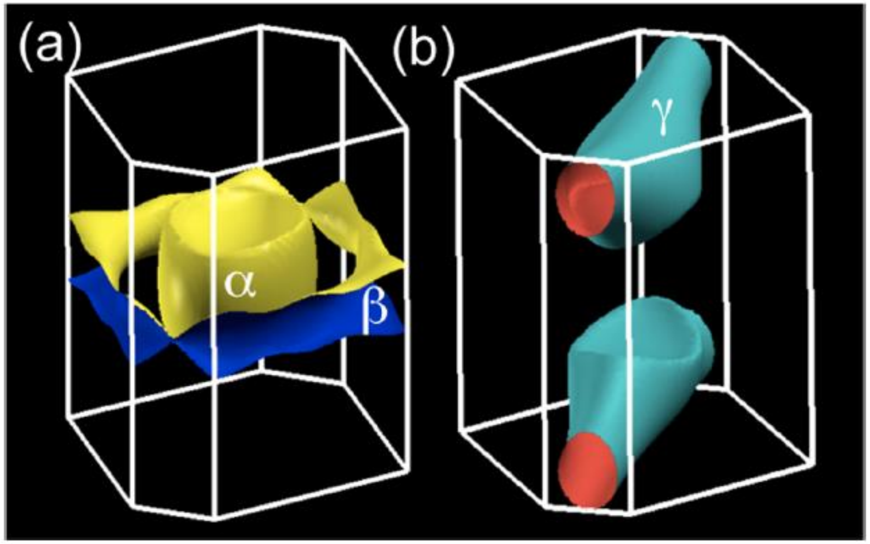
Charge:
>SC at 24 K

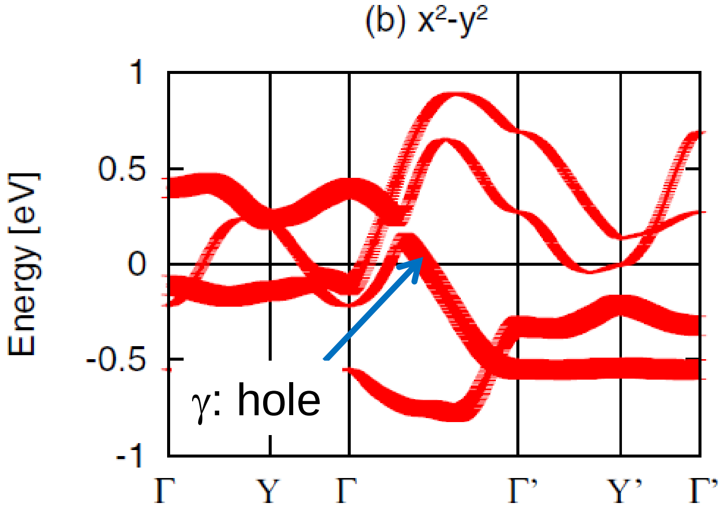
- ◆ Questions
  - ✓ Mott transition: Mott or Peierls ?
  - ✓ Magnetism: Localized or itinerant pictures? Role of orbitals?
  - ✓ SC: Spin, orbital, and charge fluctuations? *s*+- or *d* wave?
  - ✓ Substitution effect: Carrier dopant or scatter?

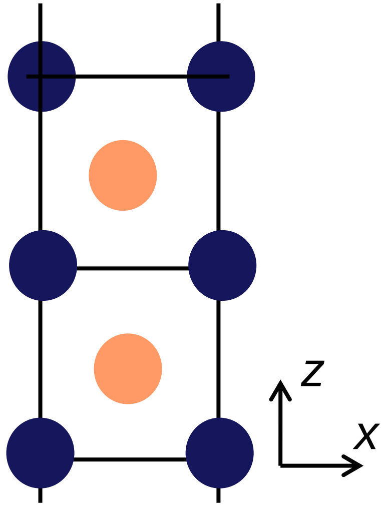
First principle calculation by Arita

P = 0









- *xz*, strong correlation
- Spin fluctuations => *s*+- between α and β
- *xy* and *yz*, irrelevant

Arita, Ikeda, Sakai, Suzuki, PRB (2015); Suzuki, Arita, Ikeda, PRB (2015).

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  - ✓Basic physical properties
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- Other possible parent materials $BaFe_2Se_3$, $CsFe_2Se_3$
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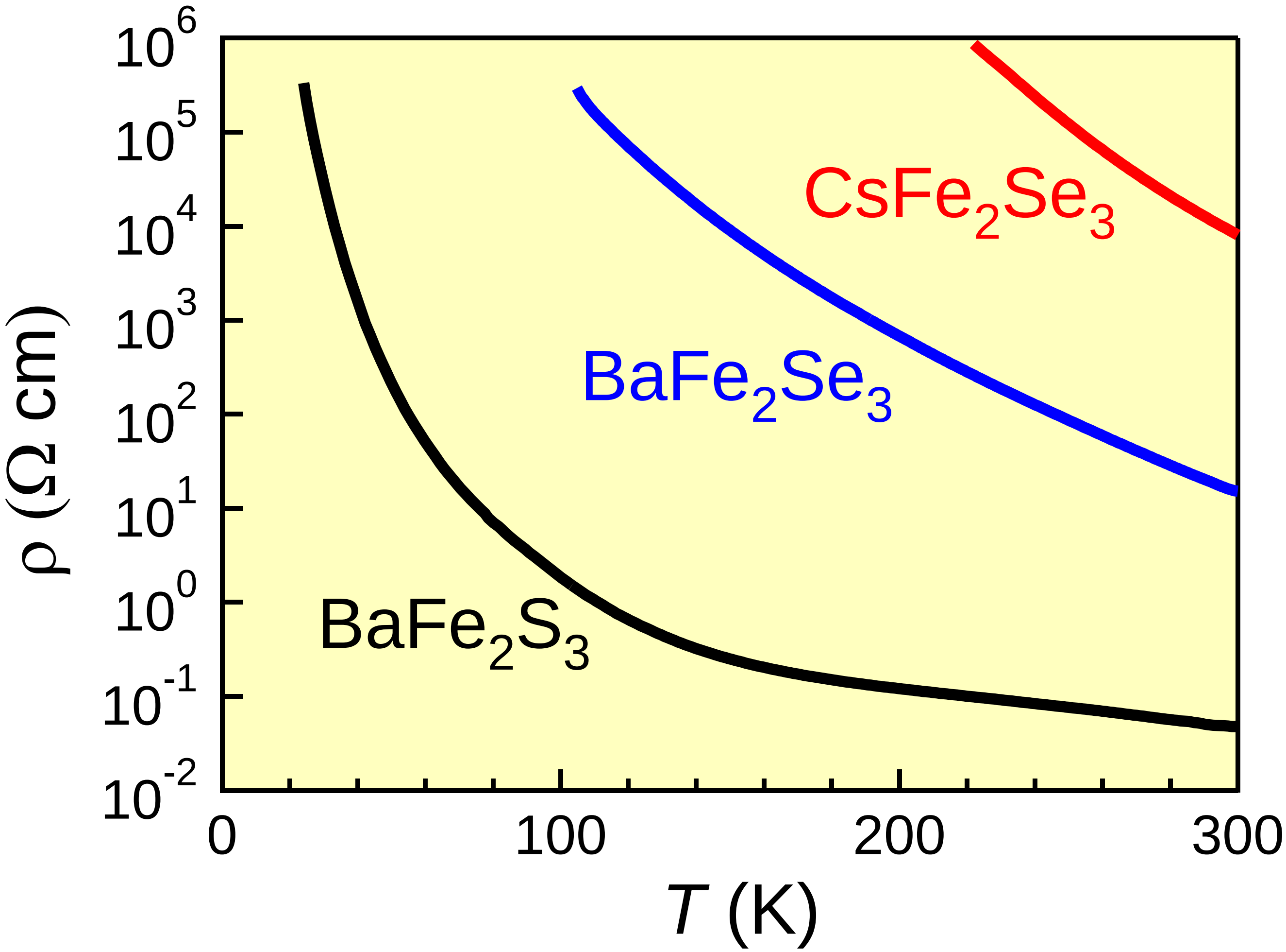
Resistivity



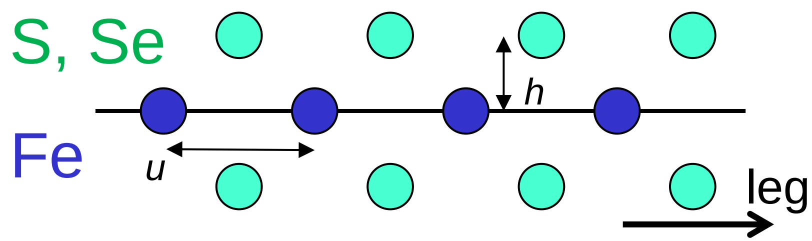
- Ba-S < Ba-Se. Unusual chemical trend.
- Mixed valence materials (Cs) > Integer valence material (Ba).

Electronic structures

$BaFe_2X_3$: $(3d)^6$

- Ionic radius: Se > S

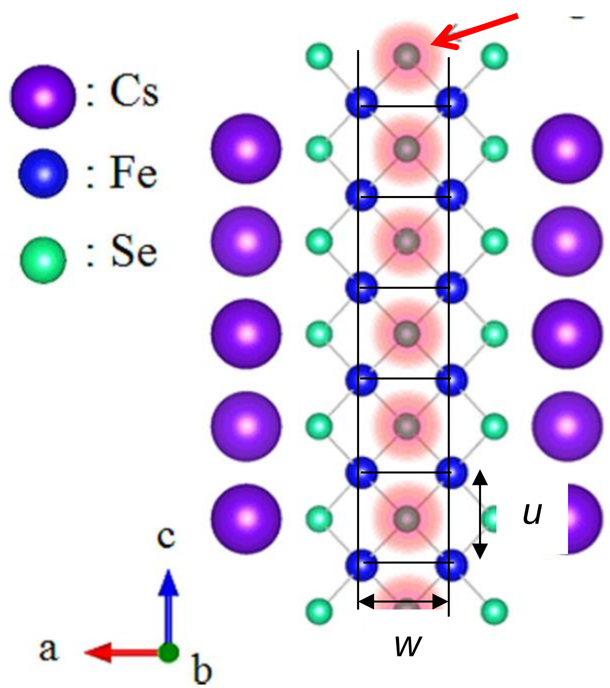
→ Bandwidth: S > Se



nm	Ba-S	Ba-Se	Rb-Se	Cs-Se
u	0.264	0.271	0.281	0.284
w	0.269	0.270	0.276	0.275
u/w	0.98	1.00	1.02	1.03

$CsFe_2Se_3$: $(3d)^{5.5}$

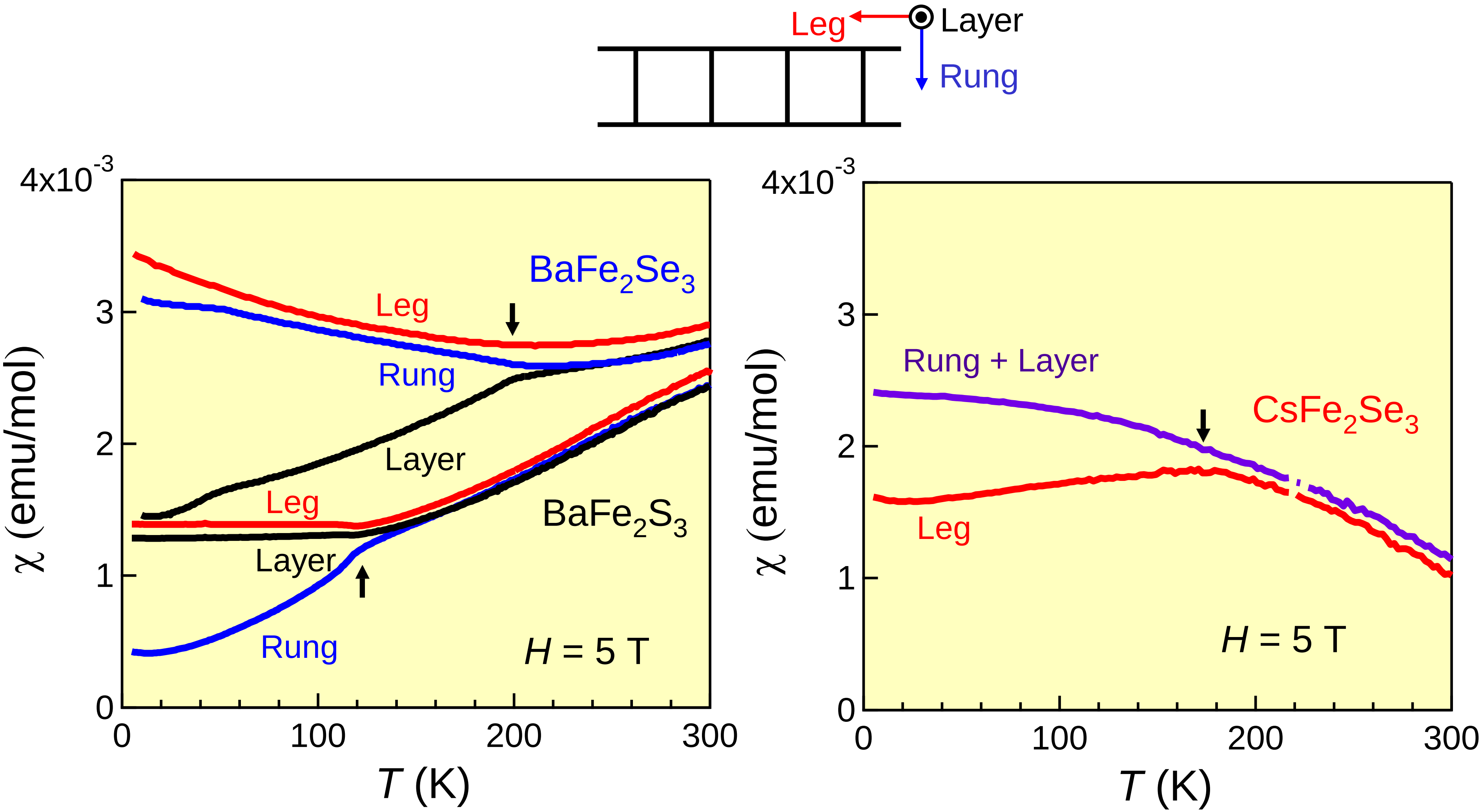
- Localized ligand holes



Ootsuki, PRB (2014).

- Resistivity: $BaFe_2S_3$ < $BaFe_2Se_3$ < $CsFe_2Se_3$.

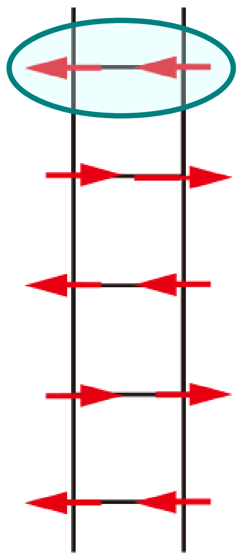
Magnetic susceptibility



- Antiferromagnetic transition with variety of the easy axis.
- Decrease in χ on cooling in A = Ba due to 1D or itinerant origin.
- Weak ferromagnetism in $CsFe_2Se_3$.

Magnetic structure

$BaFe_2S_3$



Stripe

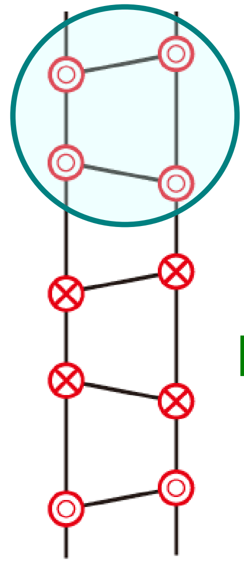
Cmcm

ψ_1

1.3 μ_B

110 K

$BaFe_2Se_3$



Block

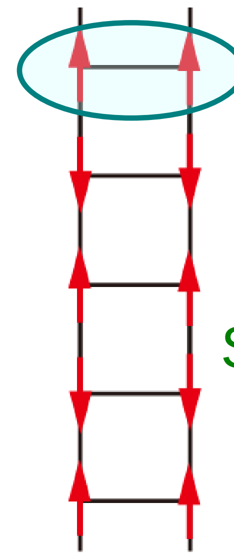
Pnma

$\Psi_{4, 10, 16, 22}$

2.8 μ_B

255 K

$CsFe_2Se_3$



Stripe

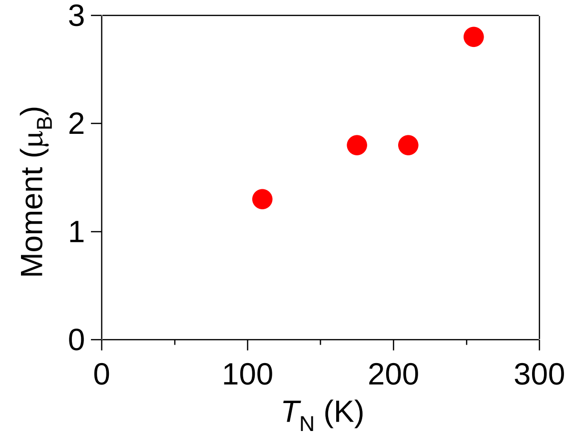
Cmcm

$\psi_9 + (\psi_{7, 8})$

1.8 μ_B

175 K

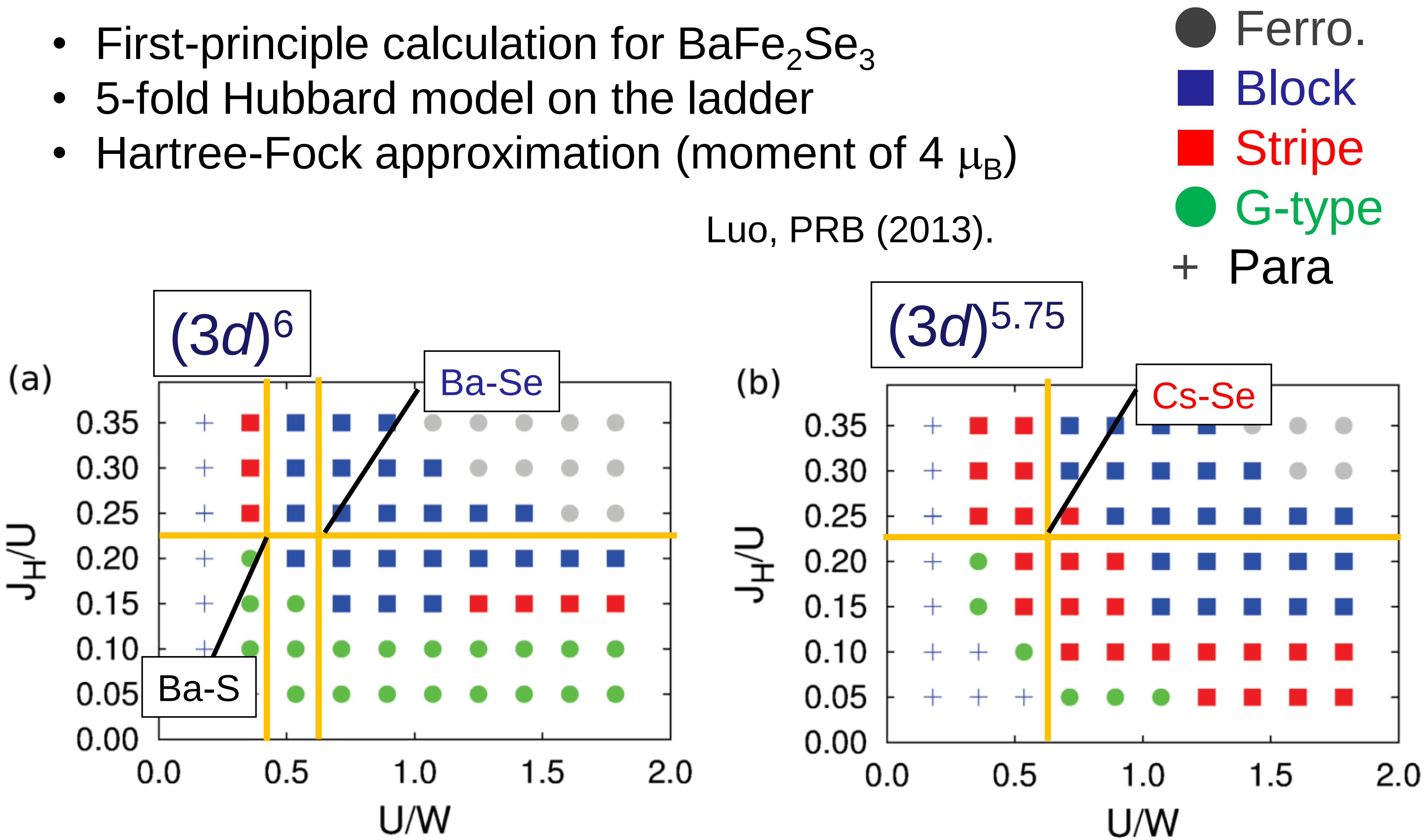
- Wide variety of magnetic order.
- Magnetic moment scales with T_N.



Global phase diagram by Dagotto

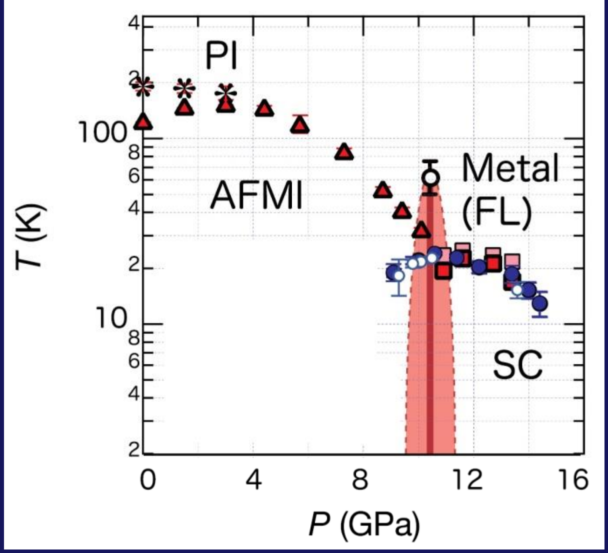
- First-principle calculation for $BaFe_2Se_3$
- 5-fold Hubbard model on the ladder
- Hartree-Fock approximation (moment of 4 μ_B)

Luo, PRB (2013).



- Intermediate coupling, *U/W* ~ 0.5.
- Parent materials for new high-T_c superconductors.

Summary: $BaFe_2S_3$



- **Mott physics**
  - 1 D ladder lattice
  - Stripe magnetic order
  - Orbital order?
  - Mott transition with dimensional crossover
  - Superconductivity with T_c = 24 K
- **Relevance to cuprates and organic SC**
- **Non-toxic Fe-based superconductors**

Nambu, KO, PRB (2012). Du, KO, PRB (2012). Du, KO, PRB (2014).
Ootsuki, Mizokawa, KO, PRB (2015). Hawai, Sato, KO, PRB (2015).
Takahashi, KO, Nat. Mater. (2015). Hirata, KO, PRB (2015).
Yamauchi, KO, PRL (2015).