A review of recent evidences of orbital-selective Mott physics in Fe-based superconductors

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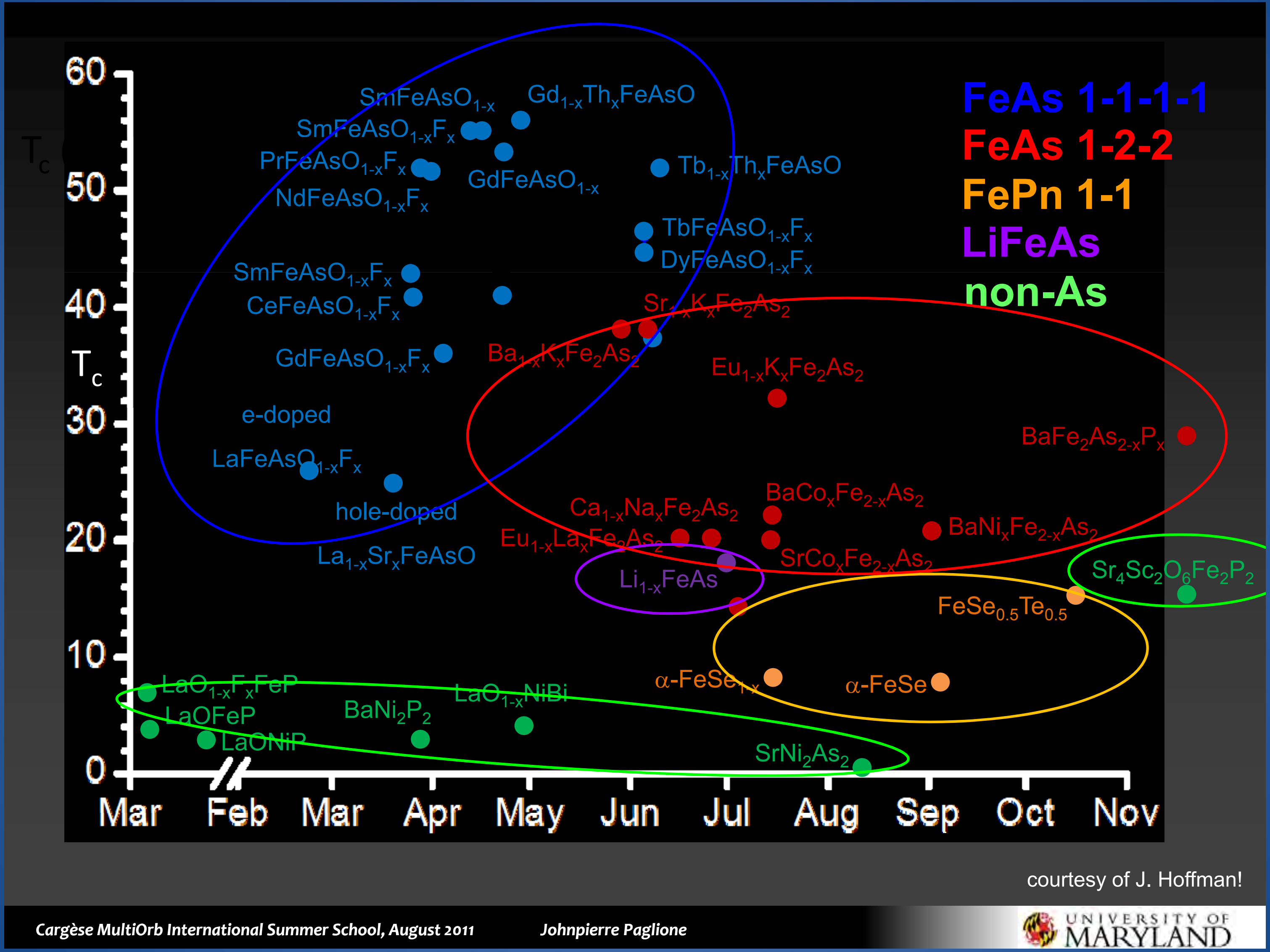
ESPCI ParisTech

SPICE Workshop on Bad Metal Behaviour in Mott Systems
29.06.2015 Mainz

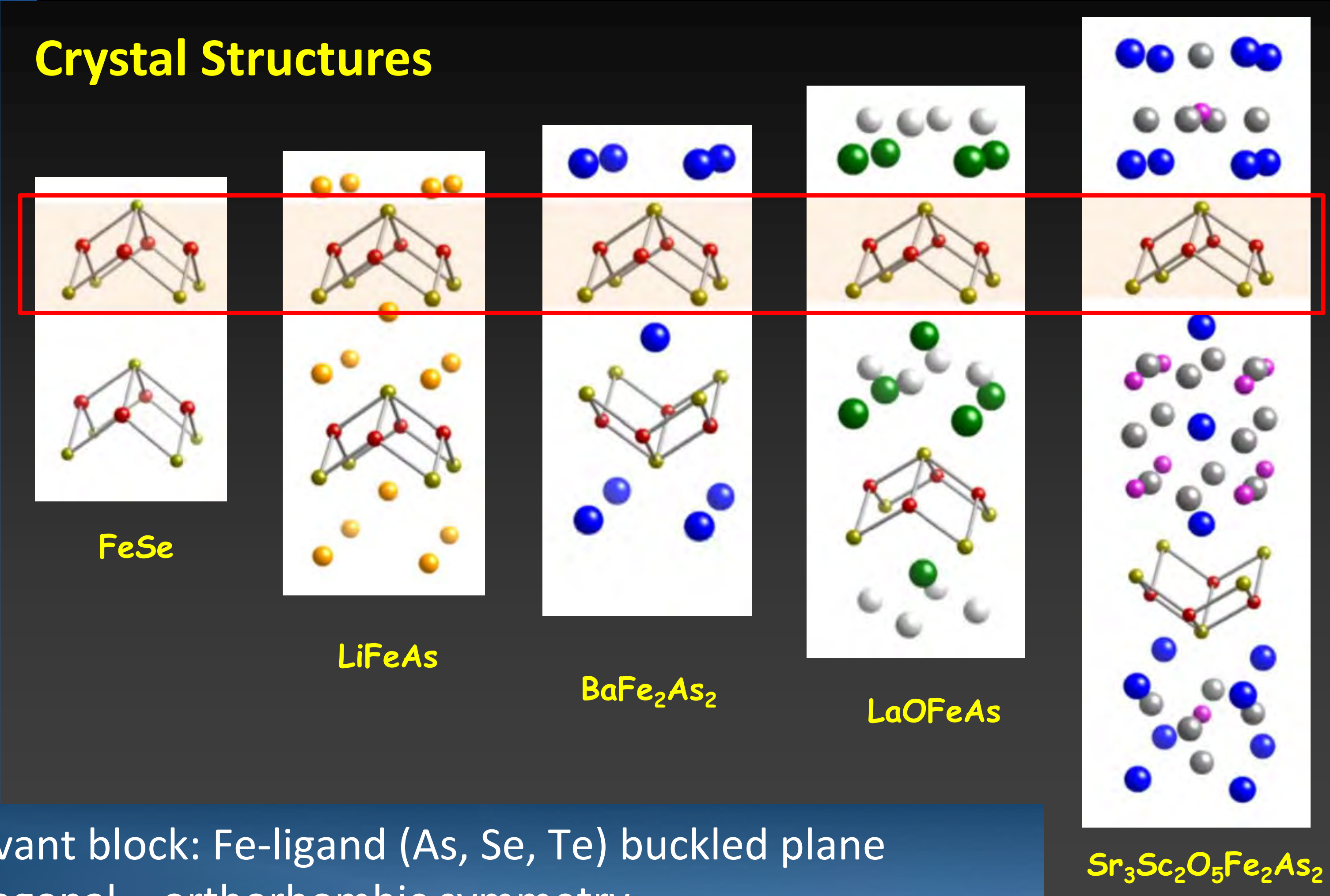
Iron-based superconductors



courtesy of J. Hoffman!

Cargèse MultiOrb International Summer School, August 2011 *Johnpierre Paglione*

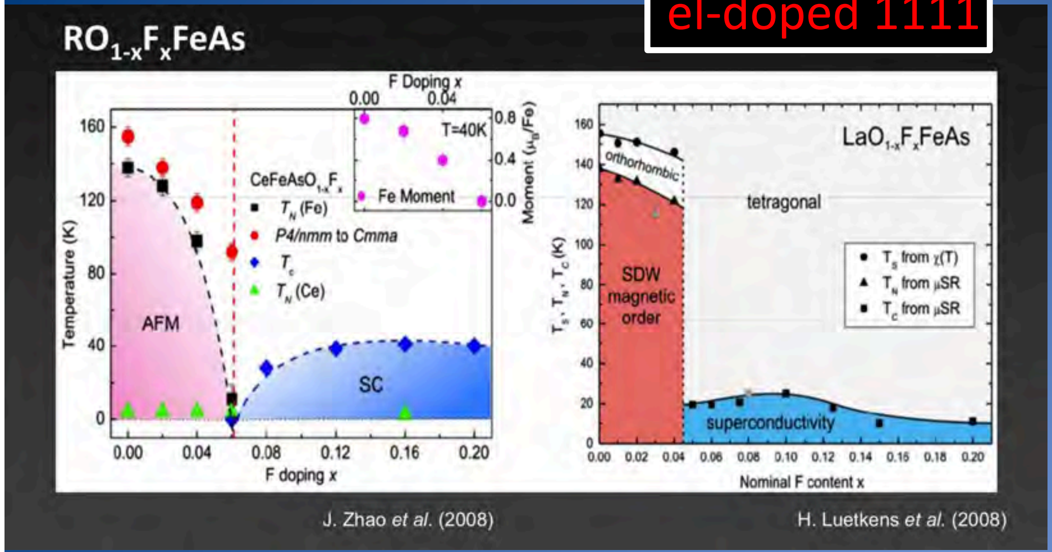
Iron-based superconductors



Paglione/Greene review (2010)

- relevant block: Fe-ligand (As, Se, Te) buckled plane
- tetragonal – orthorhombic symmetry

el-doped 1111



J. Zhao *et al.* (2008)

H. Luetkens *et al.* (2008)

hole-doped 122

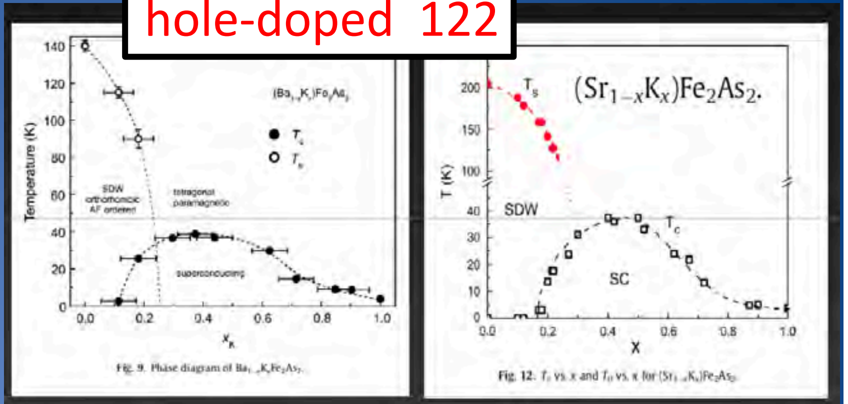
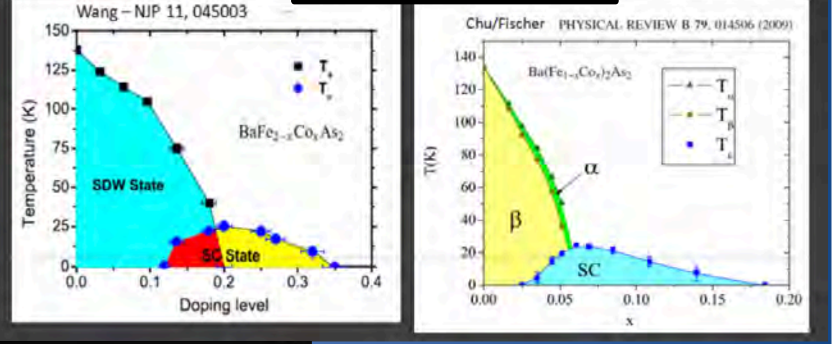


Fig. 9. Phase diagram of Ba$_{1-x}$K$_x$Fe$_2$As$_2$.

Fig. 12. T_c vs. x and T_0 vs. x for (Sr$_{1-x}$K$_x$)Fe$_2$As$_2$.

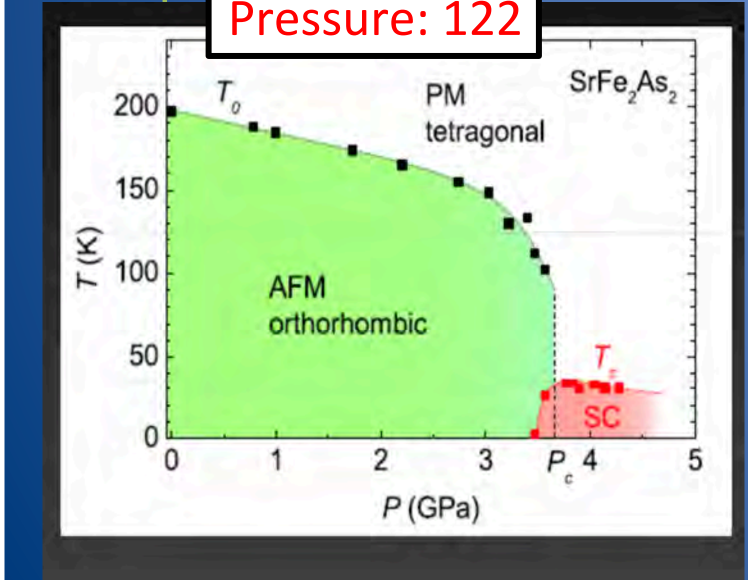
el-doped 122



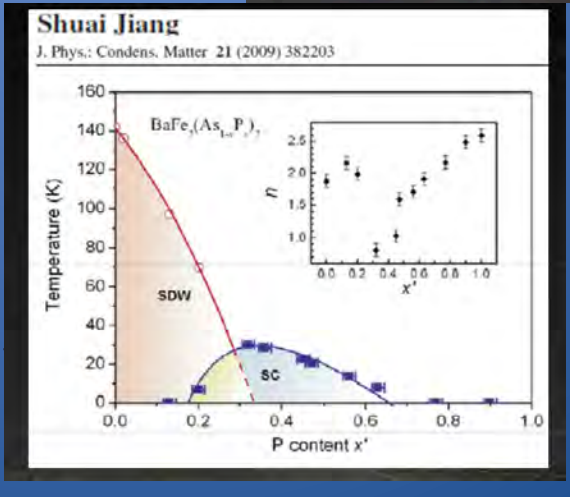
Wang – NJP 11, 045003

Chu/Fischer PHYSICAL REVIEW B 79, 014506 (2009)

Pressure: 122



H. Kotegawa *et al.* (2008)

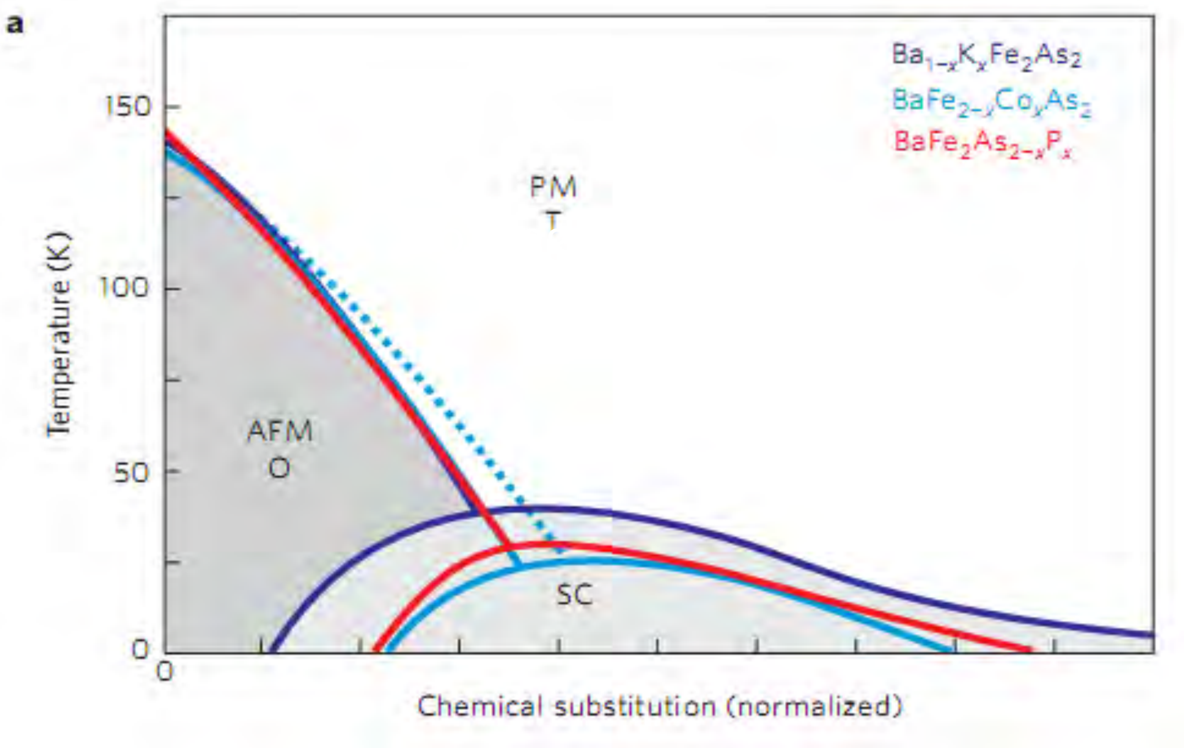


Shuai Jiang

J. Phys.: Condens. Matter **21** (2009) 382203

Isovalent doping: 122

hole-doped 122

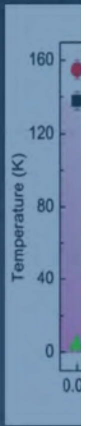


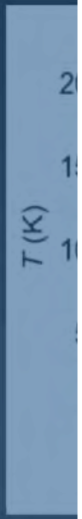
Paglione and Greene, NatPhys2010

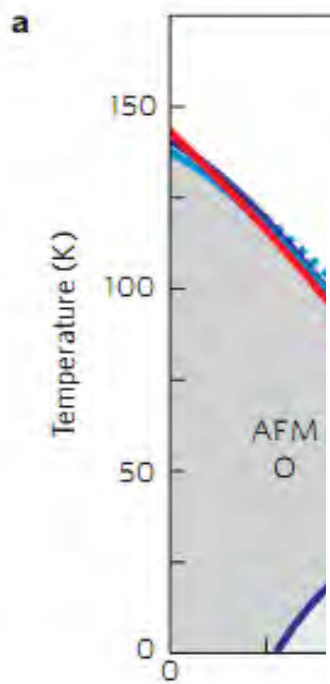
H. Kotegawa *et al.* (2008)

hole-doped 122

RO_{1-}

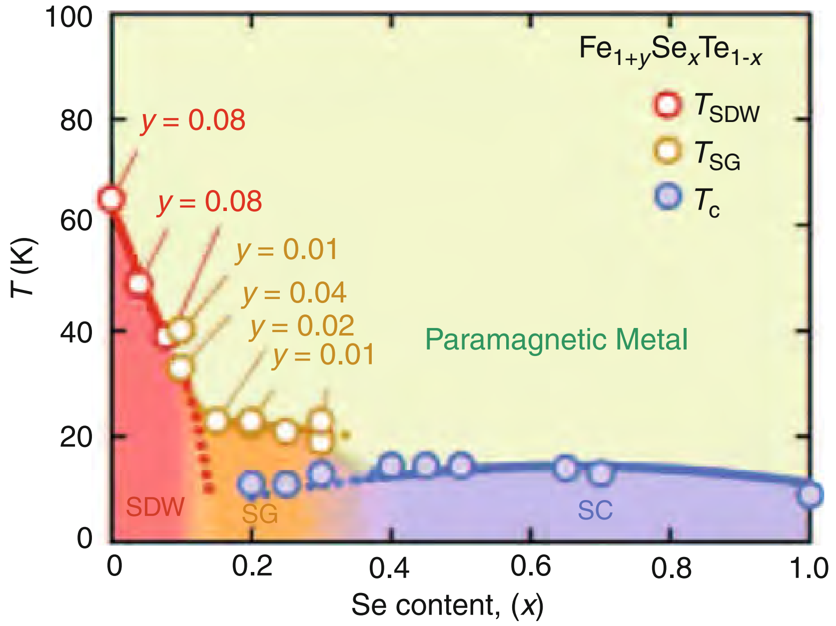




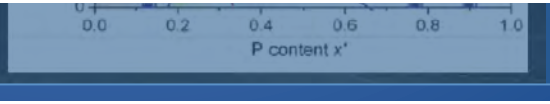


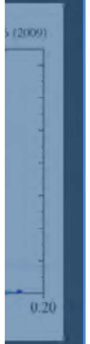
Pagli

No magnetic transition in FeSe



H. Kotegawa *et al.* (20





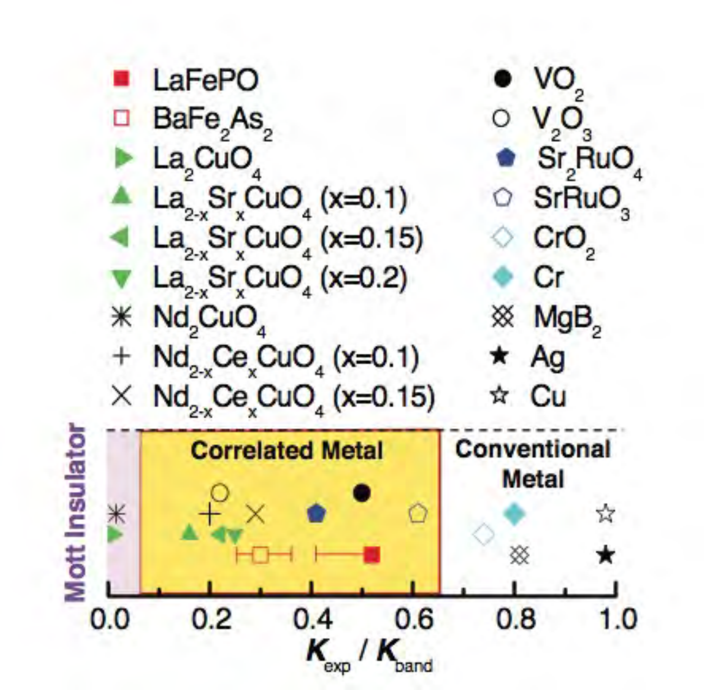
Correlations in Iron SC?

Contrasting evidences for correlation strength

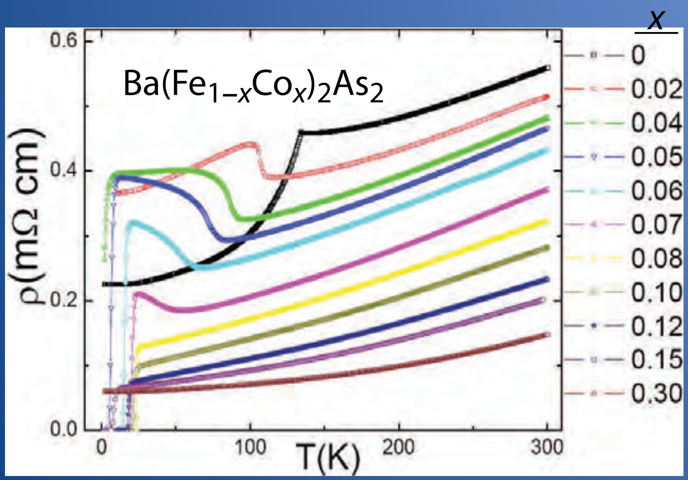
weak
- no Mott insulator in the phase diagram
- hard detection of any Hubbard bands
- moderate correlations from Optics

strong
- bad metallicity
- strong sensitivity to doping
- local vs itinerant magnetism

Weak-coupling vs Strong-coupling scenarios



Qazilbash et al. NatPhys2009



Fang et al. PRB80 (2009)
Rullier-Albenque et al. PRL103 (2009)

Specific heat (mJ/ mol K^2)

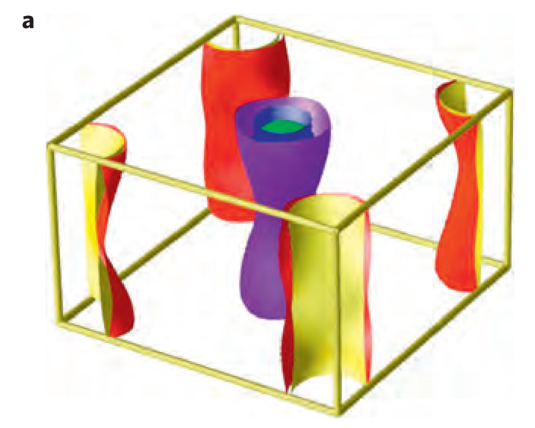
LaFePO	7
$Ba(Co_xFe_{1-x})_2As_2$	15-20
$Ba_{1-x}K_xFe_2As_2$	50
$FeSe_{0.88}$	9.2
KFe_2As_2	69-102
$K_{0.8}Fe_{1.6}Se_2$	6

Review: Stewart, RMP (2011)

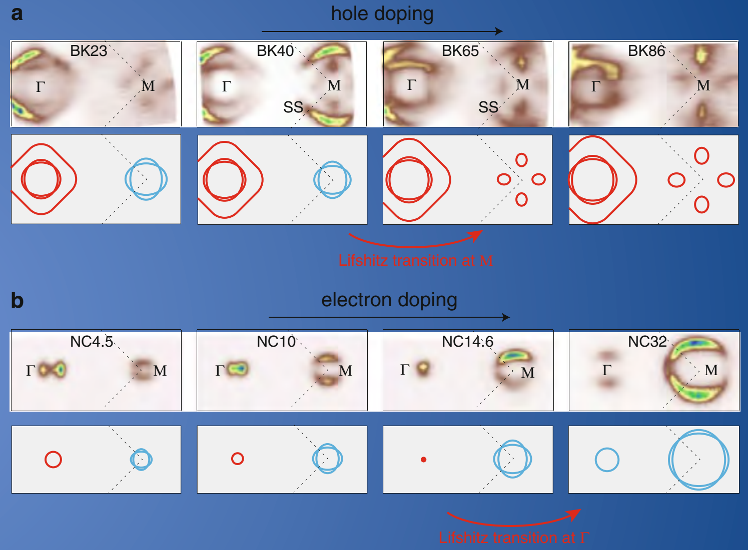
Theoretical approaches: itinerant electrons

- multi-orbital: 5 bands (Fe 3d) at the Fermi level (W~4eV)
  n=6 conduction electrons
- Partially lifted degeneracy (crystal-field splitting ~0.4eV)

Mazin and Schmalian, Physica C 2009

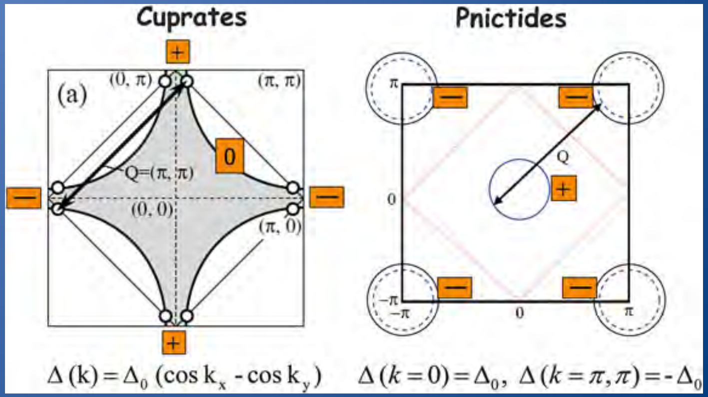


Zhang et al. ,
Springer Book 2015



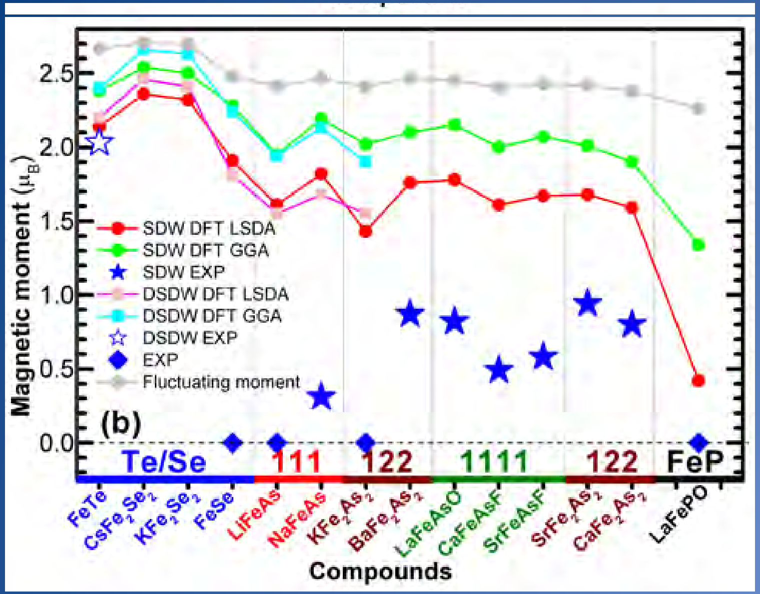
Itinerant electrons:

- DFT gives correct FS topology (semi-compensated metal)
- Nesting of FS pockets provides SDW and spin-fluctuations induce SC pairing ($S^{\pm}$-wave)

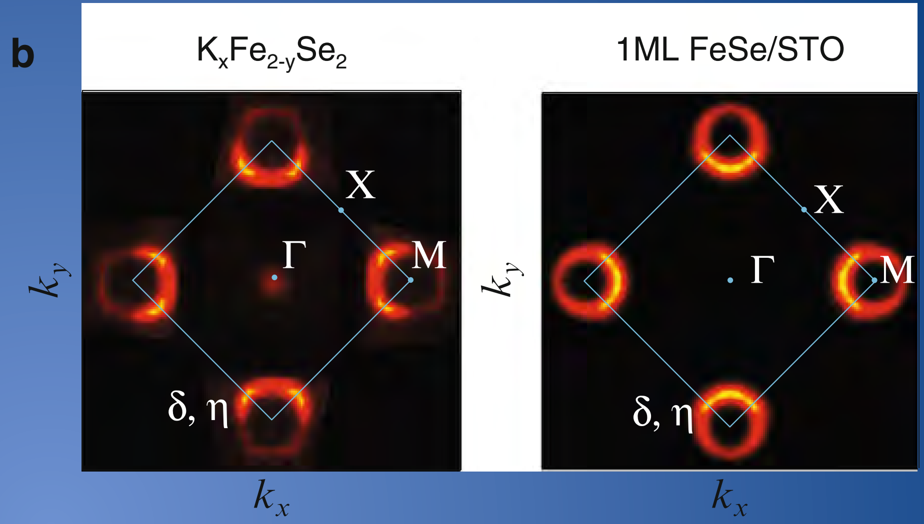


A. Chubukov, Springer Book 2015

Problems of the itinerant model

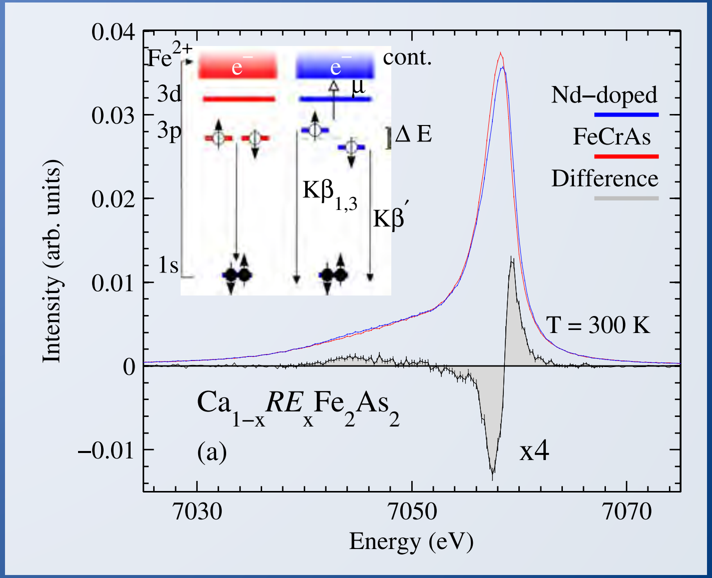


Zhang et al. Nat Mat 10 (2011) Tan et al. Nat Mat 12 (2014)



Problems

- LDA bands 2-3 times too dispersive
- LSDA unusually overestimates the ordered magnetic moment
- FeSe (Tc=8K) and LiFeAs (Tc=18K) do not have magnetic order
- $K_xFe_{2-y}Se_2$ (Tc~40K) and FeSe monolayer (Tc=109K??) only have electron pockets. KFe_2As_2 (Tc=4K) only hole pockets.
- Direct evidence of local moments in the PM phase (XES)



XES: Gretarsson et al. PRB 2011

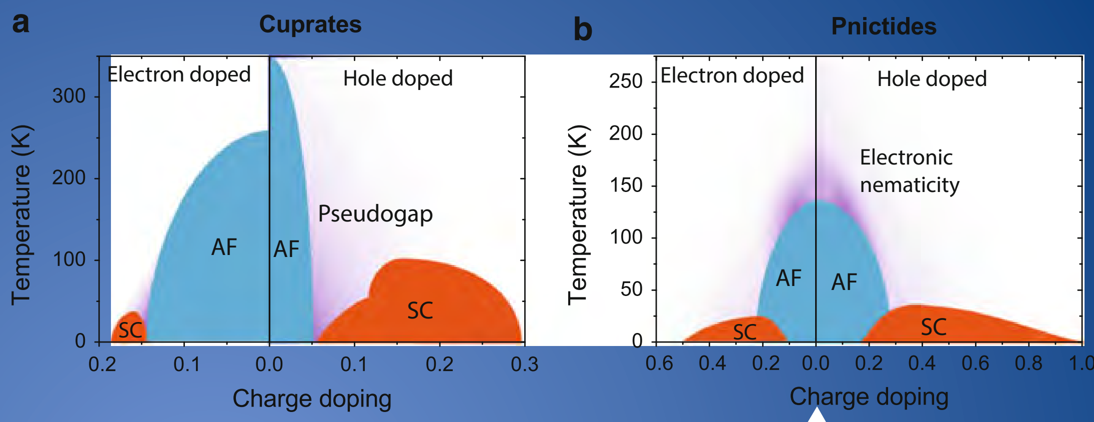
Localized electrons?

Analogy with cuprates led to theories based on the t-J (J_1-J_2) model:

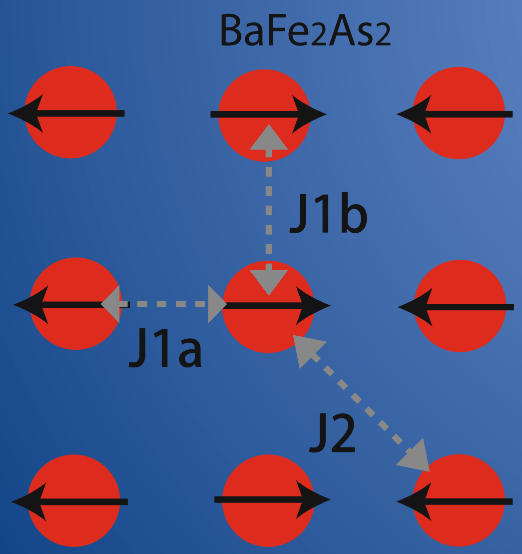
- Good magnetic order

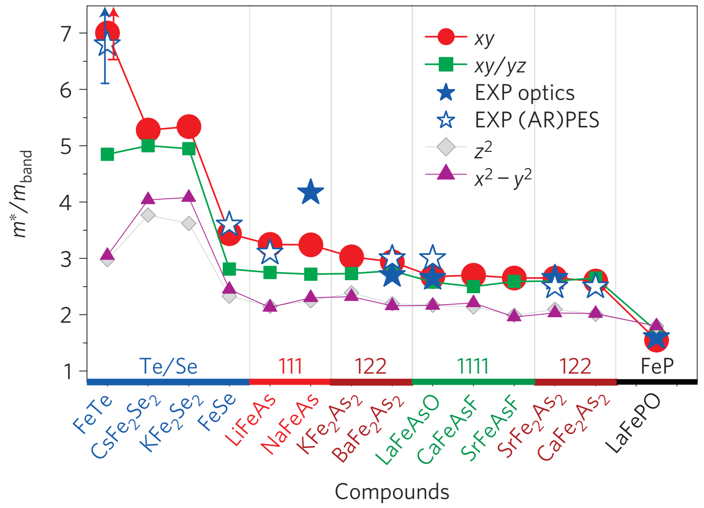
Problems:

- Ad hoc (metal)
- superconductivity?



No Mott insulator here!





Yin et al, Nat Mat 10 (2011)

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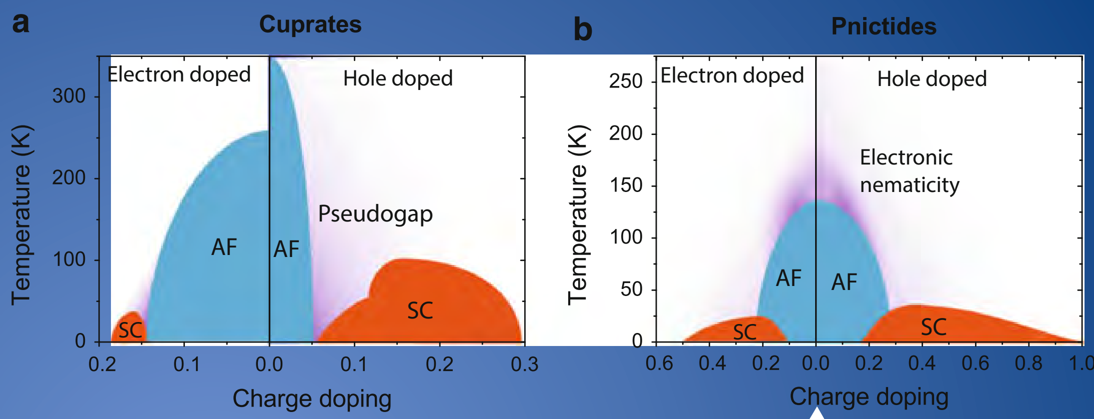

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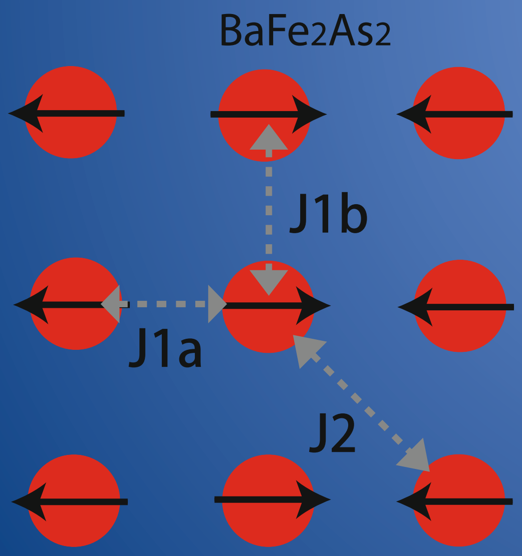


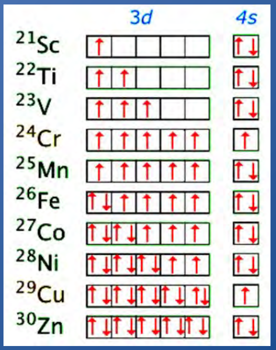
DMFT *et similia*

$$H=\sum_{k} H_k^{DFT} \quad +U\sum_{i,m} n_{im\uparrow}n_{im\downarrow}$$

(U'=U-2J)

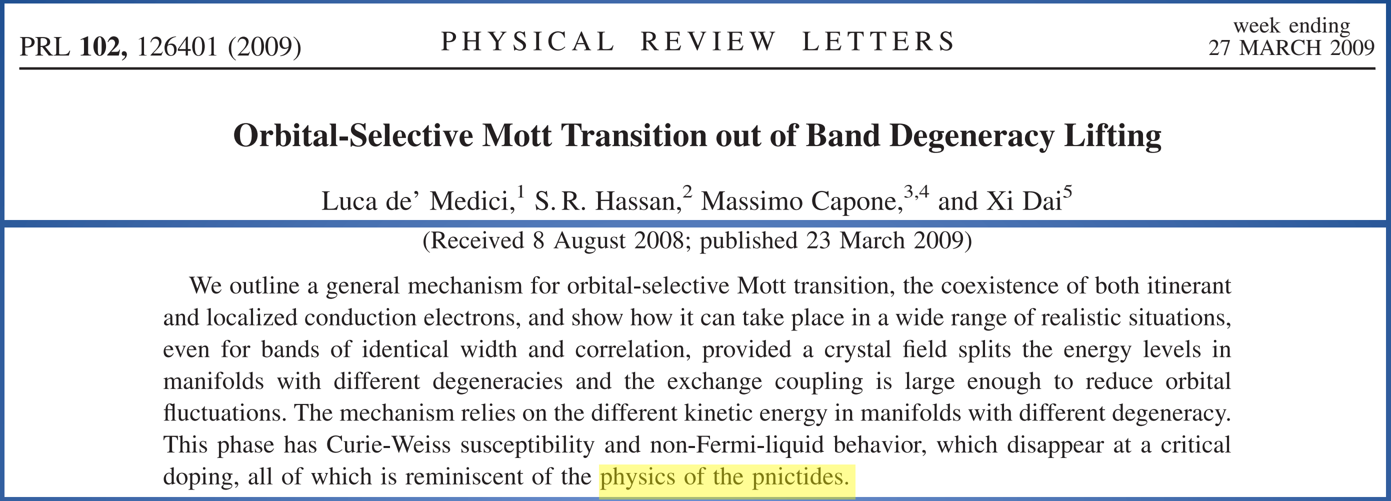
$$+U'\sum_{i,m>m',\sigma} n_{im\sigma}n_{im'\bar{\sigma}}+(U'-J)\sum_{i,m>m',\sigma} n_{im\sigma}n_{im'\sigma}$$

Interactions
U~2-4eV
J~0.4eV
(W~4eV)



Nearly half-filled 3d-shells: Hund's coupling important!

Selective Mott Physics



PRL **102,** 126401 (2009) PHYSICAL REVIEW LETTERS week ending 27 MARCH 2009

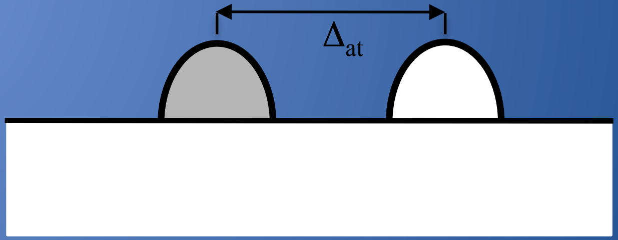
Orbital-Selective Mott Transition out of Band Degeneracy Lifting

Luca de' Medici,[1] S. R. Hassan,[2] Massimo Capone,[3,4] and Xi Dai[5]

(Received 8 August 2008; published 23 March 2009)

We outline a general mechanism for orbital-selective Mott transition, the coexistence of both itinerant and localized conduction electrons, and show how it can take place in a wide range of realistic situations, even for bands of identical width and correlation, provided a crystal field splits the energy levels in manifolds with different degeneracies and the exchange coupling is large enough to reduce orbital fluctuations. The mechanism relies on the different kinetic energy in manifolds with different degeneracy. This phase has Curie-Weiss susceptibility and non-Fermi-liquid behavior, which disappear at a critical doping, all of which is reminiscent of the physics of the pnictides.

Mechanism: Hund's induced orbital decoupling



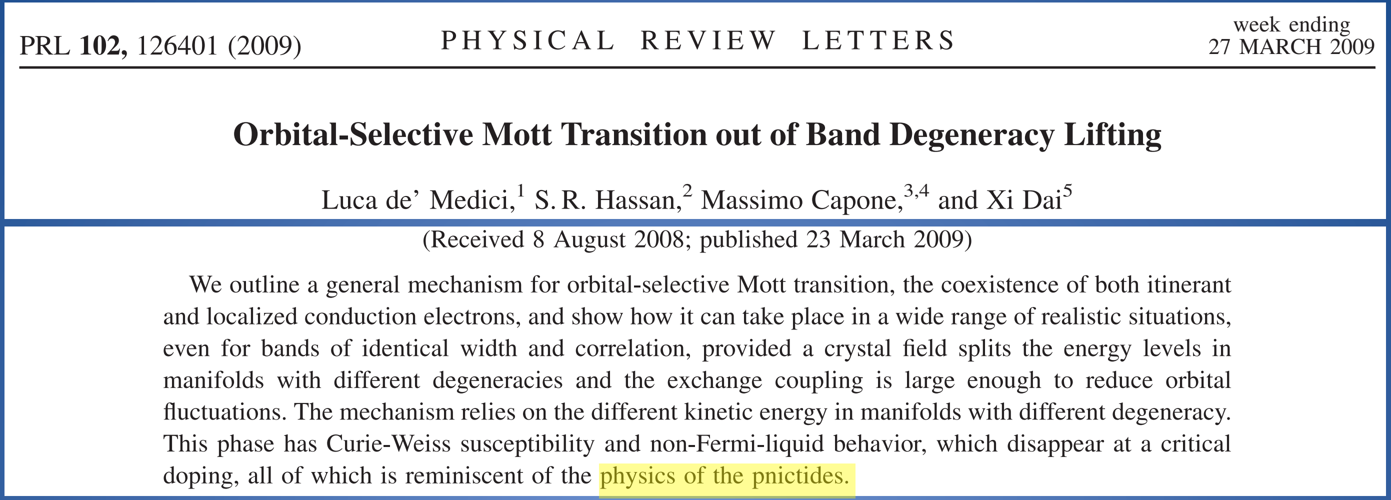
See also

LdM, PRB 83, 205112 (2011)

LdM, "Weak *and* strong correlations in Fe superconductors", vol 211, pp 409-441

In *Iron-based Superconductivity*, Springer 2015

Selective Mott Physics



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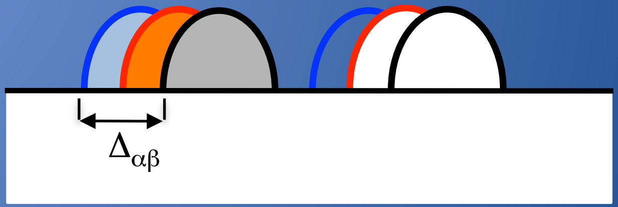

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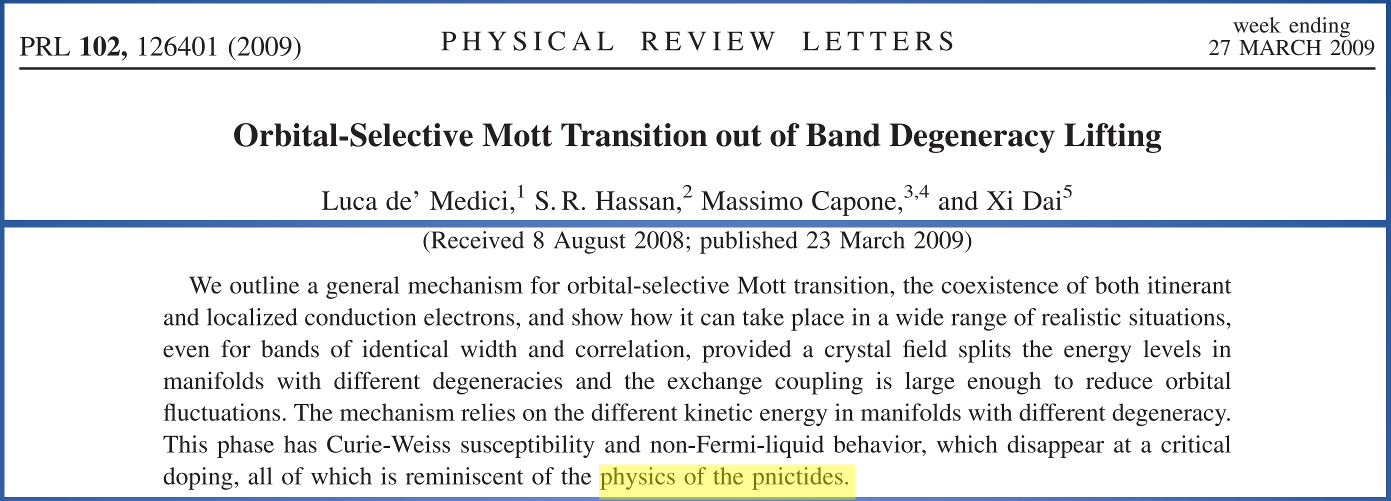

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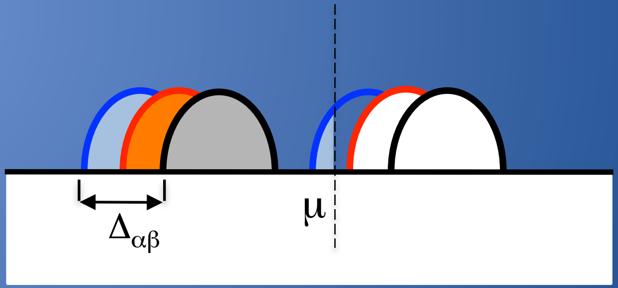

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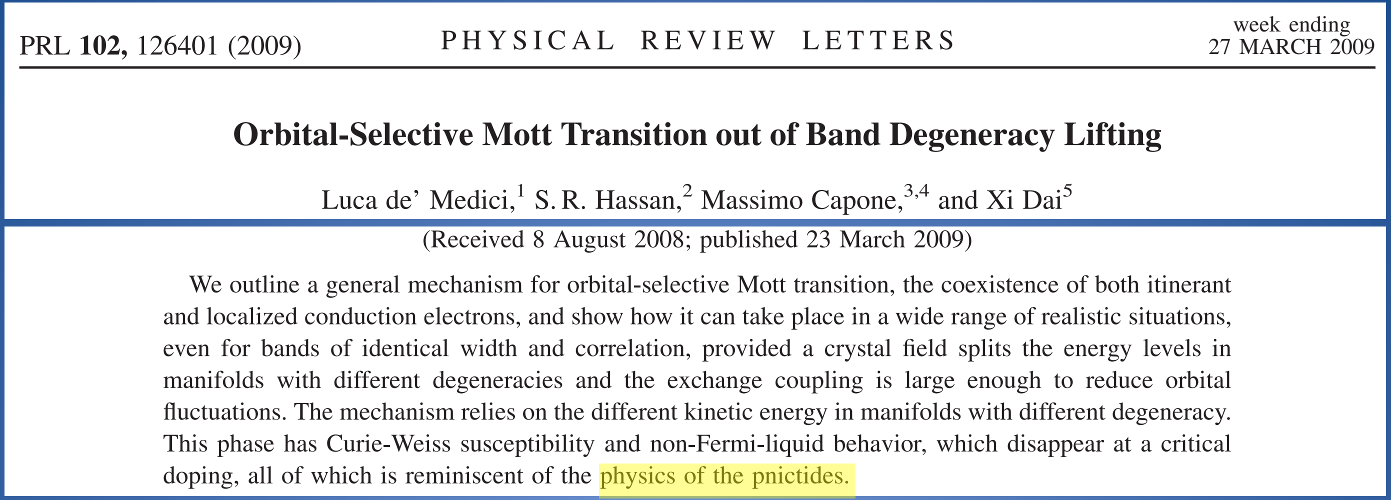

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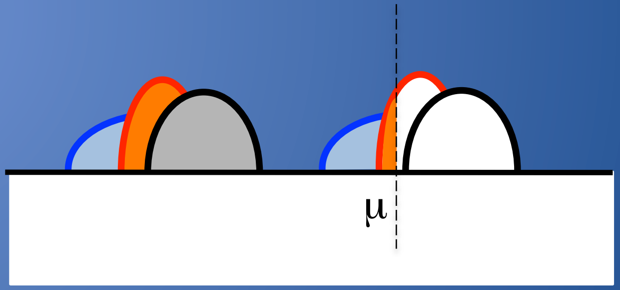

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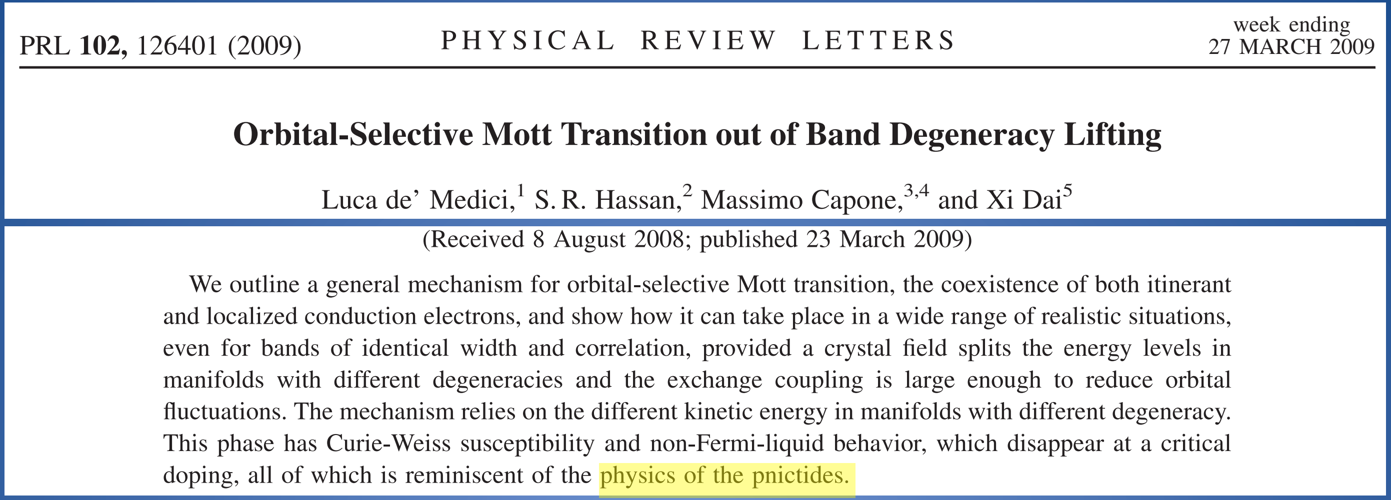

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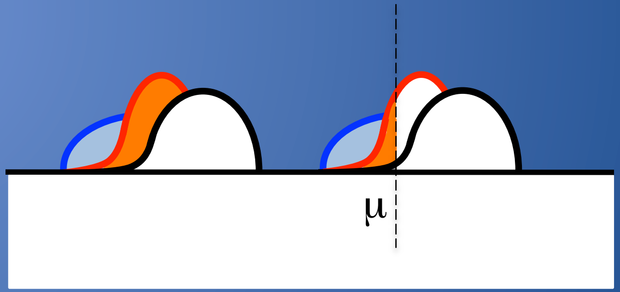

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In *Iron-based Superconductivity*, Springer 2015

Phenomenological scenarios based on coexisting itinerant/localized electrons:

A. Hackl and M. Vojta, New J. Phys.11, 055064 (2009)

Kou et al. Europhys. Lett. 88, 17010 (2009)

Yin W.G. et al., Phys. Rev. Lett.105, 107004(2010)

Orbital Selectivity: early experimental indications

Optical conductivity

- A. Lucarelli, et al., New J. Phys. **12**, 073036 (2010)……………………… Co-122
- N.L. Wang et al., J. Phys. Condens. Matter **24**, 294202 (2012)……. K-122, Co-122

Magnetoresistance

- H.Q. Yuan et al., arXiv e-prints ………….(2011)……………………………. Co-122

ARPES

- A. Tamai et al. Phys. Rev. Lett. **104**, 097002 (2010)……………………… FeTeSe
- W. Malaeb, et al., Phys. Rev. B **86**, 165117 (2012)……………………… K-122

EPR and NMR

- D. Arcon, et al, Phys. Rev. B **82**, 140508 (2010)………………………….. FeTeSe

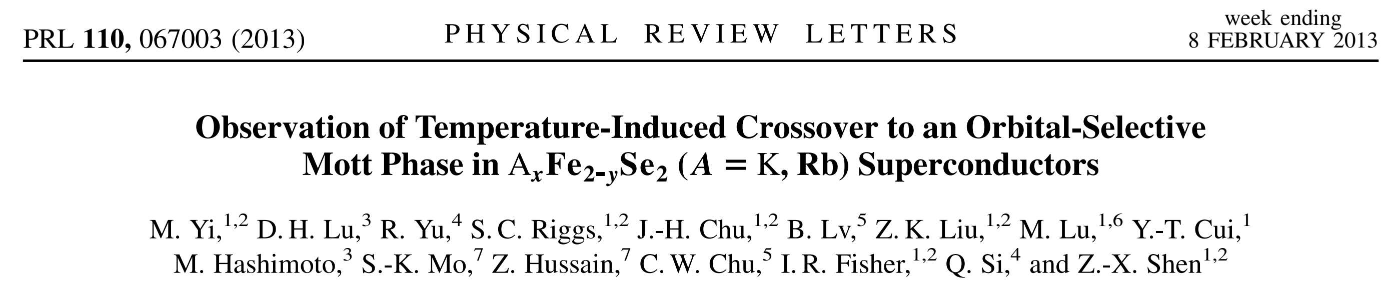
NEUTRONS

- Z. Xu et al., Phys. Rev. B **84**, 052506 (2011)………………………………. FeTeSe

XES

- H. Gretarsson et al., Phys. Rev. B **84**, 100509 (2011) …………………. 122- 11- 111-245

Recent OS Mott Experimental Evidences in Fe-chalc

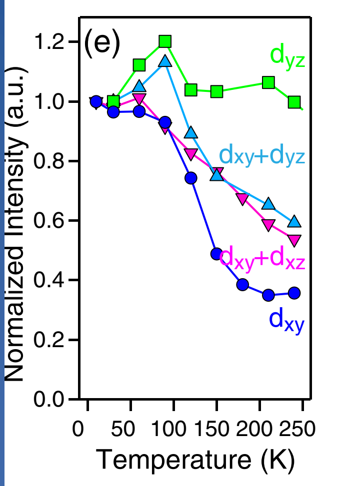


PRL **110,** 067003 (2013) PHYSICAL REVIEW LETTERS week ending 8 FEBRUARY 2013

Observation of Temperature-Induced Crossover to an Orbital-Selective Mott Phase in $A_xFe_{2-y}Se_2$ (A = K, Rb) Superconductors

M. Yi,[1,2] D. H. Lu,[3] R. Yu,[4] S. C. Riggs,[1,2] J.-H. Chu,[1,2] B. Lv,[5] Z. K. Liu,[1,2] M. Lu,[1,6] Y.-T. Cui,[1]
M. Hashimoto,[3] S.-K. Mo,[7] Z. Hussain,[7] C. W. Chu,[5] I. R. Fisher,[1,2] Q. Si,[4] and Z.-X. Shen[1,2]

ARPES



nature COMMUNICATIONS

Received 27 Sep 2013 | Accepted 6 Jan 2014 | Published 28 Jan 2014 DOI: 10.1038/ncomms4202

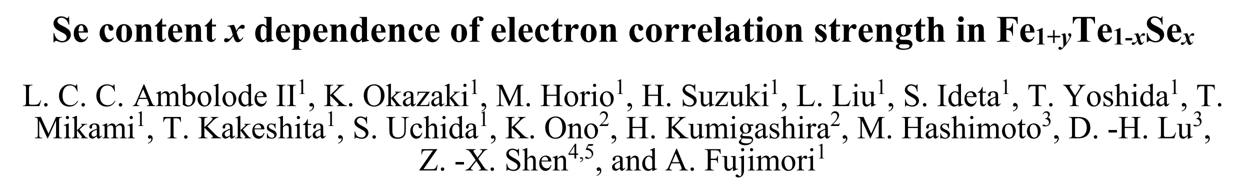
Orbital-selective metal–insulator transition and gap formation above T_C in superconducting $Rb_{1-x}Fe_{2-y}Se_2$

Zhe Wang[1], M. Schmidt[1], J. Fischer[1], V. Tsurkan[1,2], M. Greger[3], D. Vollhardt[3], A. Loidl[1] & J. Deisenhofer[1]

THz spectroscopy

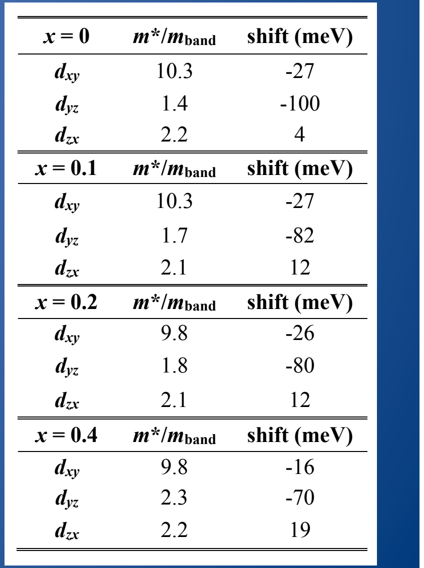
ARPES

ArXiv: 1505.07637



Se content x dependence of electron correlation strength in $Fe_{1+y}Te_{1-x}Se_x$

L. C. C. Ambolode II[1], K. Okazaki[1], M. Horio[1], H. Suzuki[1], L. Liu[1], S. Ideta[1], T. Yoshida[1], T. Mikami[1], T. Kakeshita[1], S. Uchida[1], K. Ono[2], H. Kumigashira[2], M. Hashimoto[3], D. -H. Lu[3], Z. -X. Shen[4,5], and A. Fujimori[1]



x = 0	**m^*/m_{band}**	**shift (meV)**
d_{xy}	10.3	-27
d_{yz}	1.4	-100
d_{zx}	2.2	4
x = 0.1	**m^*/m_{band}**	**shift (meV)**
d_{xy}	10.3	-27
d_{yz}	1.7	-82
d_{zx}	2.1	12
x = 0.2	**m^*/m_{band}**	**shift (meV)**
d_{xy}	9.8	-26
d_{yz}	1.8	-80
d_{zx}	2.1	12
x = 0.4	**m^*/m_{band}**	**shift (meV)**
d_{xy}	9.8	-16
d_{yz}	2.3	-70
d_{zx}	2.2	19

Also ARPES/Quantum Oscillations on FeSe monocrystal: Watson et al. PRB 91, 155106 (2015)

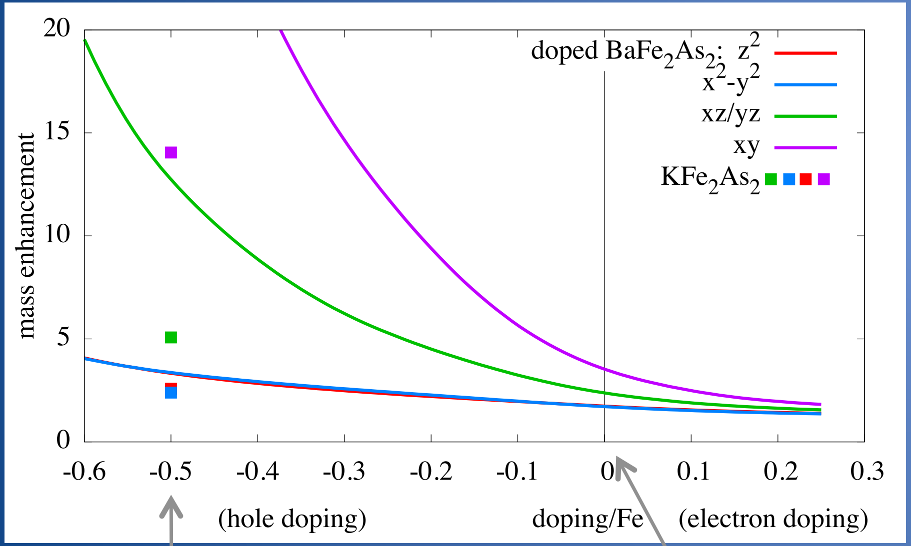
Selective Mott Physics in doped pnictides

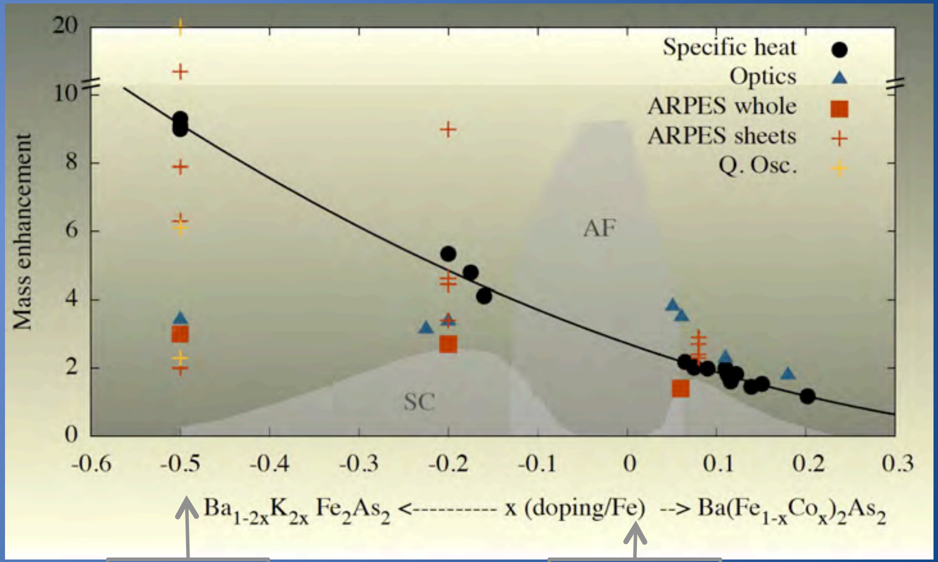
mass enhancements

LdM, G. Giovannetti, M. Capone, PRL 112, 177001 (2014)
“Selective Mott Physics as a Key to Iron Superconductors”

Theory (LDA+Slave-spins)

Experimental data
(high-T tetragonal phase)





$\mathrm{KFe_2As_2}$

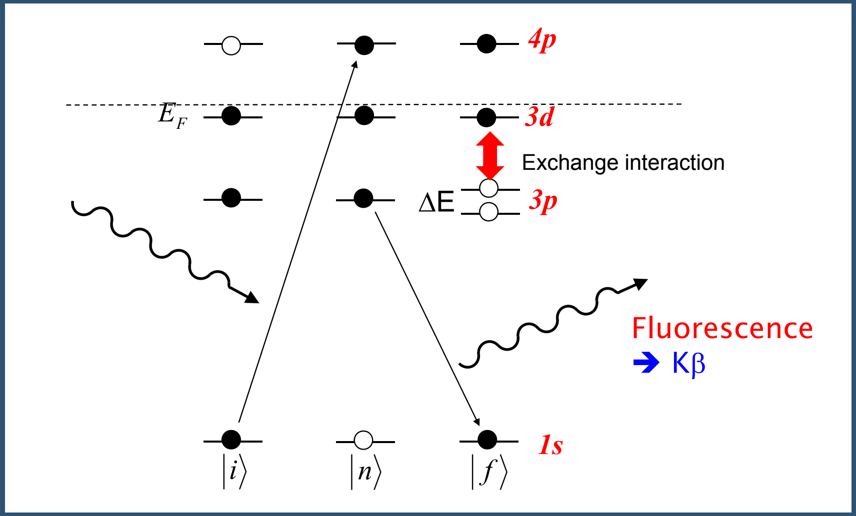
$\mathrm{BaFe_2As_2}$

$\mathrm{KFe_2As_2}$

$\mathrm{BaFe_2As_2}$

Selective correlation strength: strongly *and* weakly correlated electrons

Local moments (XES) develop with hole-doping in 122



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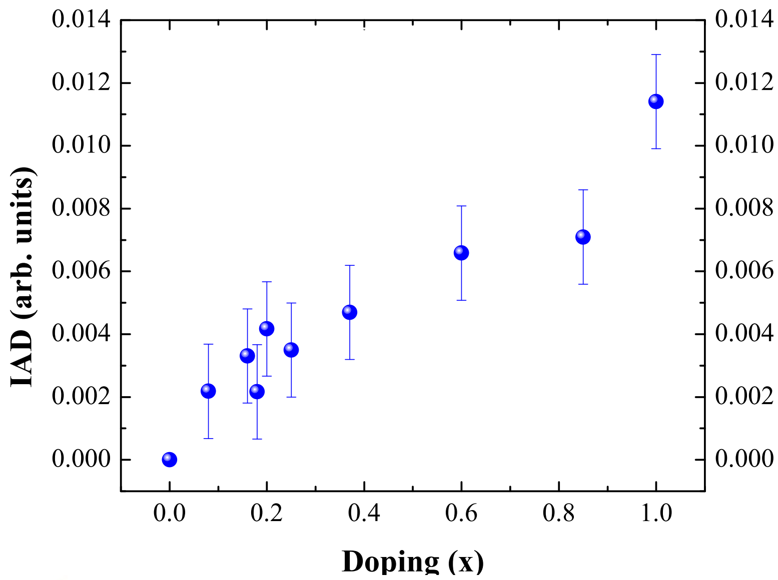
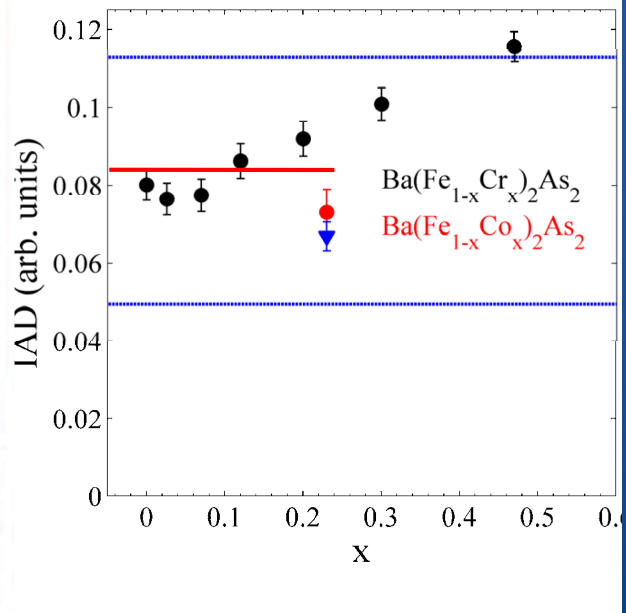




Instantaneous local moments building with hole-doping in 122 Fe-pnictides!

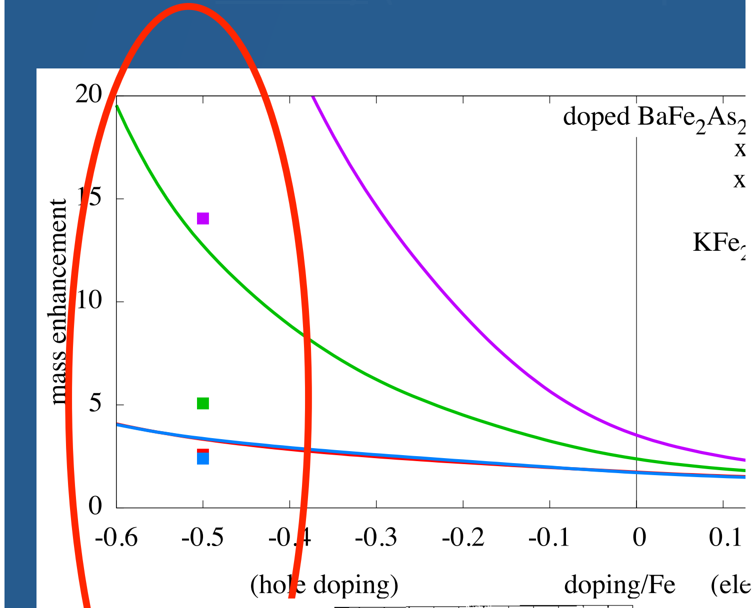
S. Lafuerza, H. Gretarsson et al., unpublished

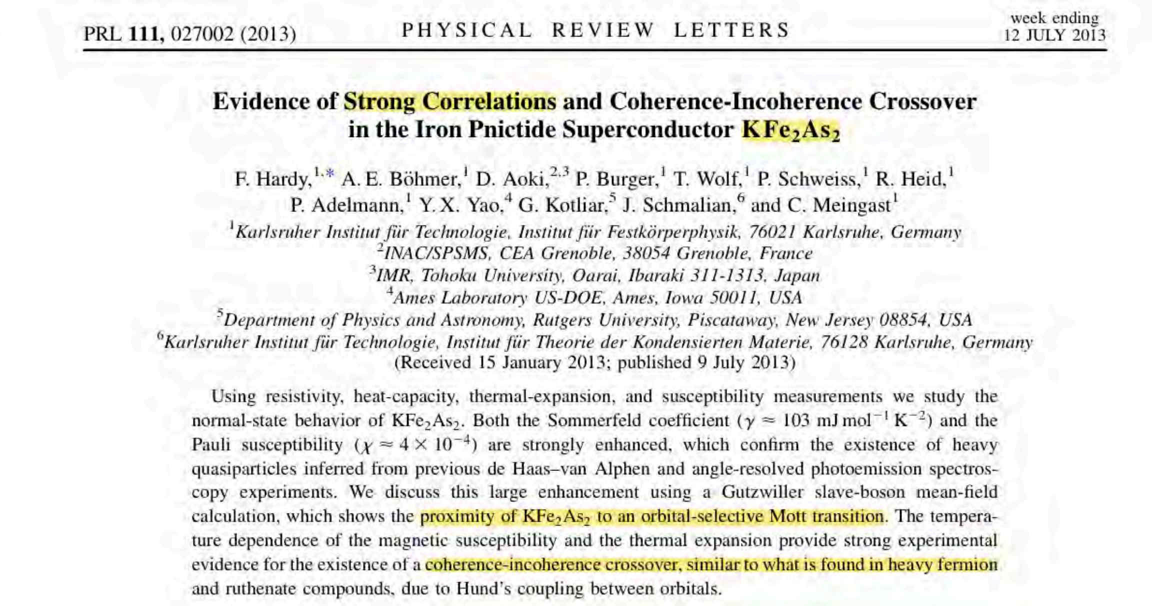
Selective Mott Physics in doped pnictides

mass enhancements

Theory (LDA+Slave-spins)

Experimental data





PRL **111,** 027002 (2013) PHYSICAL REVIEW LETTERS week ending 12 JULY 2013

Evidence of Strong Correlations and Coherence-Incoherence Crossover in the Iron Pnictide Superconductor KFe_2As_2

F. Hardy,[1,*] A. E. Böhmer,[1] D. Aoki,[2,3] P. Burger,[1] T. Wolf,[1] P. Schweiss,[1] R. Heid,[1]
P. Adelmann,[1] Y. X. Yao,[4] G. Kotliar,[5] J. Schmalian,[6] and C. Meingast[1]
[1]*Karlsruher Institut für Technologie, Institut für Festkörperphysik, 76021 Karlsruhe, Germany*
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[3]*IMR, Tohoku University, Oarai, Ibaraki 311-1313, Japan*
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[5]*Department of Physics and Astronomy, Rutgers University, Piscataway, New Jersey 08854, USA*
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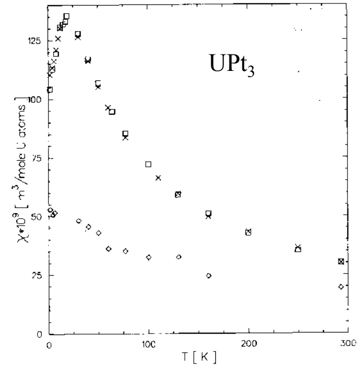
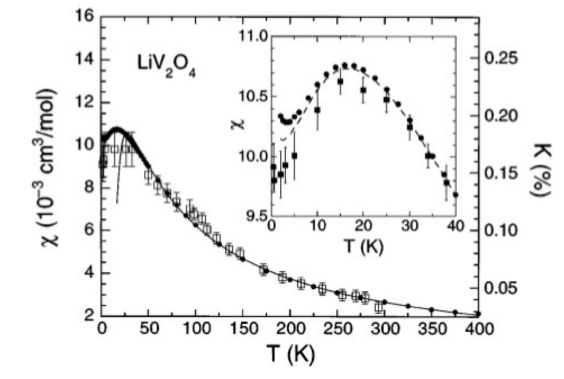
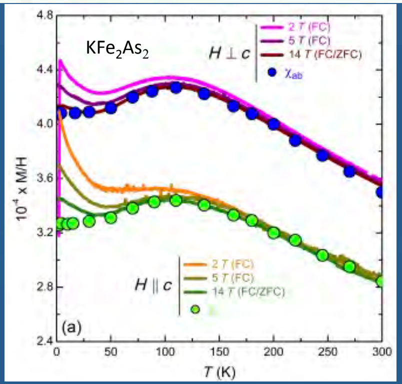
(Received 15 January 2013; published 9 July 2013)

Using resistivity, heat-capacity, thermal-expansion, and susceptibility measurements we study the normal-state behavior of KFe_2As_2. Both the Sommerfeld coefficient ($\gamma \approx 103$ mJ mol^{-1} K^{-2}) and the Pauli susceptibility ($\chi \approx 4 \times 10^{-4}$) are strongly enhanced, which confirm the existence of heavy quasiparticles inferred from previous de Haas–van Alphen and angle-resolved photoemission spectroscopy experiments. We discuss this large enhancement using a Gutzwiller slave-boson mean-field calculation, which shows the proximity of KFe_2As_2 to an orbital-selective Mott transition. The temperature dependence of the magnetic susceptibility and the thermal expansion provide strong experimental evidence for the existence of a coherence-incoherence crossover, similar to what is found in heavy fermion and ruthenate compounds, due to Hund's coupling between orbitals.

KFe_2As_2



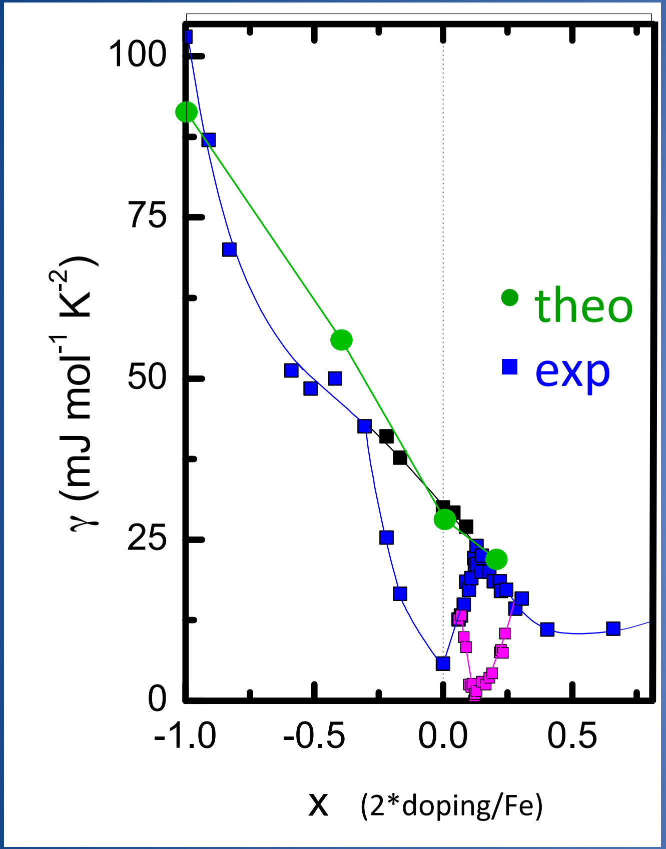




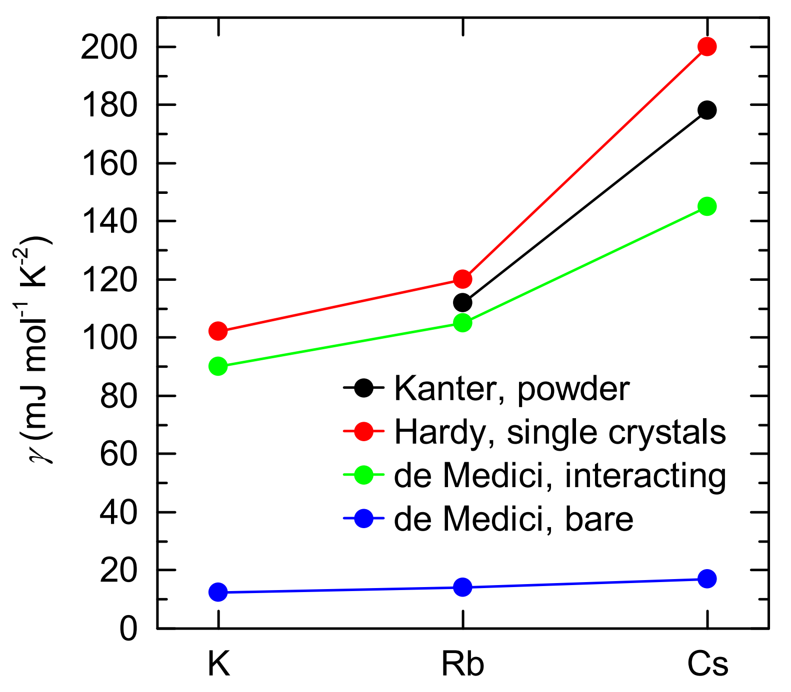
Selective

Heavy-fermionic behaviour in Fe-Superconductors

$Ba_{1-x}K_xFe_2As_2$



AFe_2As_2 (A= K, Rb, Cs)



Experiments from C. Meingast's group in Karlsruhe. F. Hardy et al. unpublished

A general mechanism for d-electron heavy-fermions

Can we also tune thermoelectric/thermomagnetic properties this way?

Coda

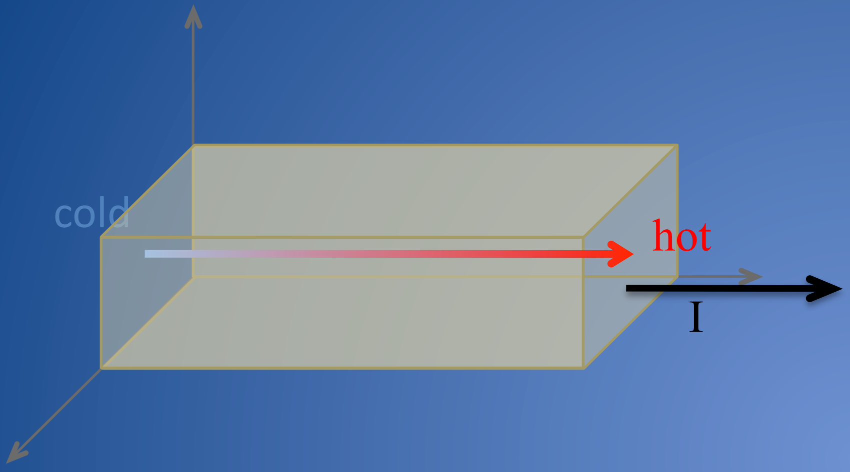
A thermomagnetic setup for self-cooling cables

Luca de' Medici – ESRF Grenoble
ESPCI ParisTech

SPICE Workshop on Bad Metal Behaviour in Mott Systems
29.06.2015 Mainz

Thermoelectric and thermomagnetic effects

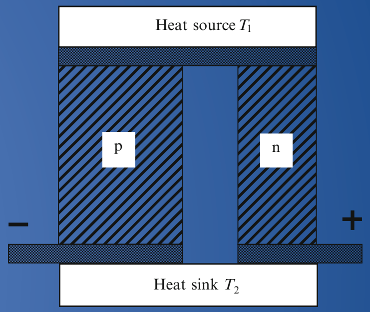
Peltier-Seebeck



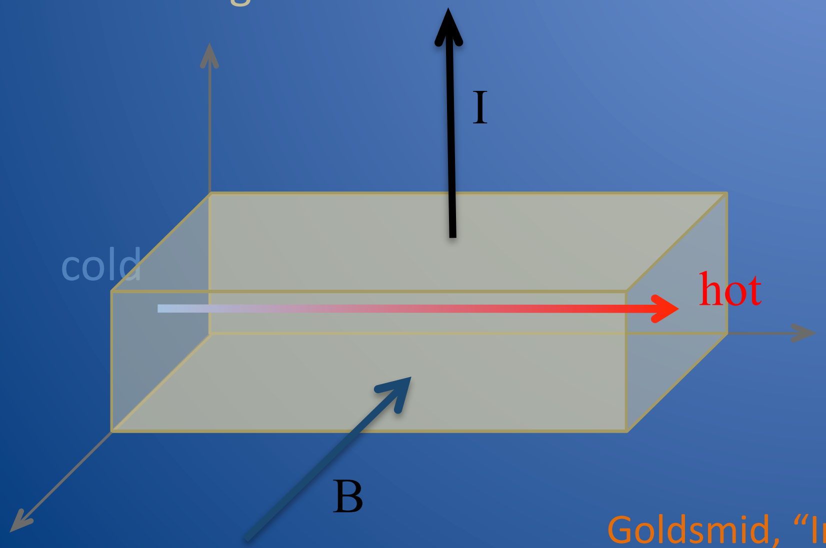
APPLICATIONS: thermocouples, peltier coolers, energy (waste heat) harvesters/converters,…

MATERIALS: Bi_2Te_3, PpTe, $FeSb_2$…

ADVANTAGES:
no magnetic field needed



Nernst-Ettingshausen



MATERIALS: Bi, Bi-Sb alloys, heavy-fermions,..

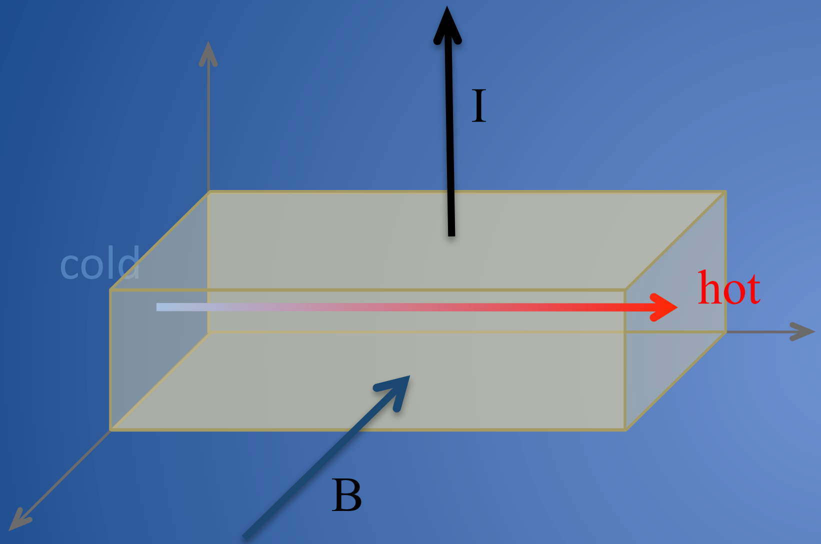
ADVANTAGES: one material is enough (no need for a couple), shaping, potentially stronger effect

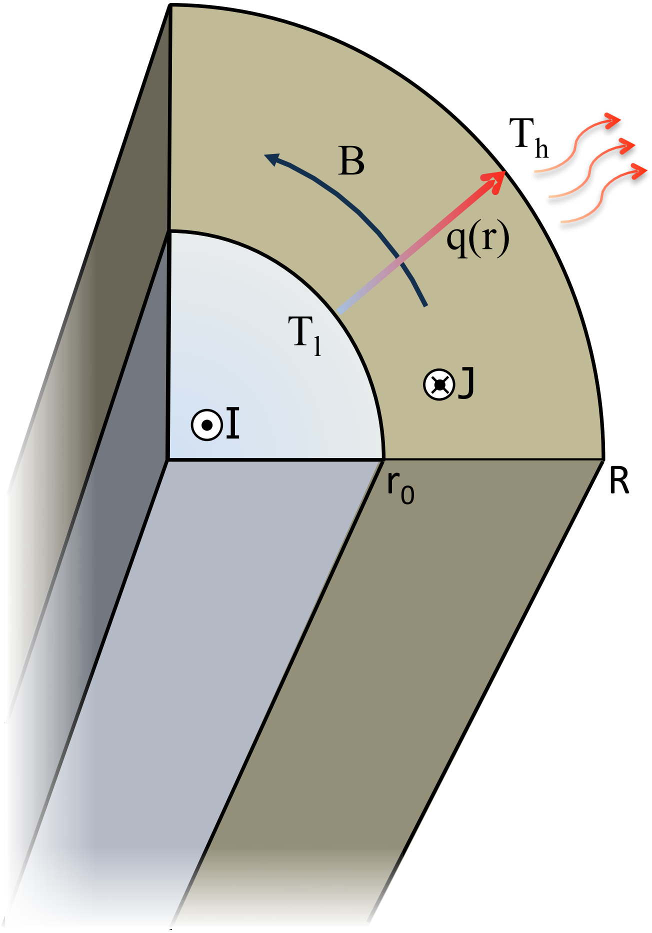
Much less studied!

Goldsmid, "Introduction to Thermoelectricity", Springer (2009)

The cable setup

LdM, ArXiv:1506.01674 (2015)





I main current transported

B magnetic field generated by I

J auxiliary current (J<<I)

Magnitude of the effect?

Ettingshausen (linear) $= NBTi_z$

Heat conduction $-K\nabla T$

Joule heat (quadratic) $\sim \rho i_z^2$

There is an optimal current for the cooling power and the efficiency, and a maximum possible ΔT

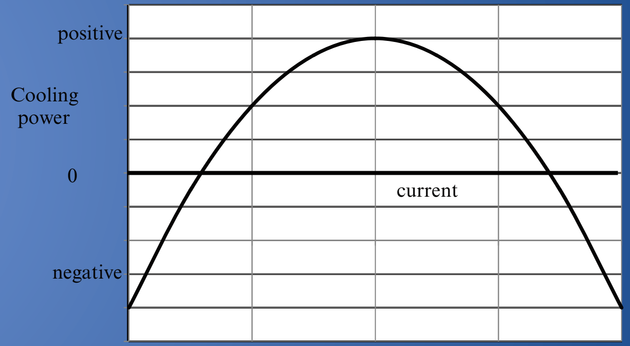
measures Ettingshausen effect

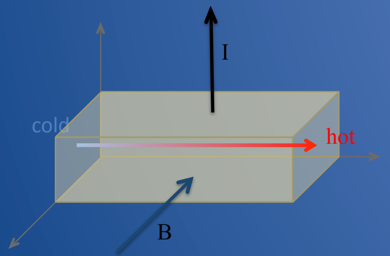
N Nernst coefficient

ρ resistivity → measures Joule effect

K thermal conductivity

measures heat backflow

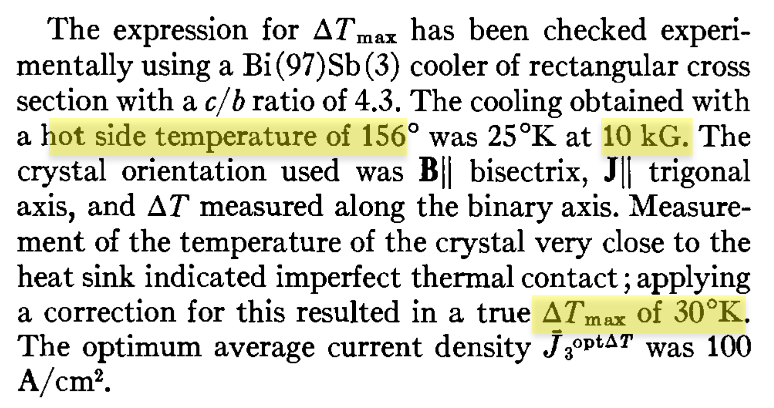




$$\Delta T_{max} = \frac{1}{2} Z T_h^2$$

for a rectangular block and constant coefficients

Thermomagnetic figure of merit [T^{-1}] $Z = \dfrac{(NB)^2}{\rho K}$



The expression for $\Delta T_{\max}$ has been checked experimentally using a Bi(97)Sb(3) cooler of rectangular cross section with a c/b ratio of 4.3. The cooling obtained with a hot side temperature of 156° was 25°K at 10 kG. The crystal orientation used was **B**‖ bisectrix, **J**‖ trigonal axis, and ΔT measured along the binary axis. Measurement of the temperature of the crystal very close to the heat sink indicated imperfect thermal contact; applying a correction for this resulted in a true $\Delta T_{\max}$ of 30°K. The optimum average current density $\bar{J}_3^{\text{opt}\Delta T}$ was 100 A/cm².

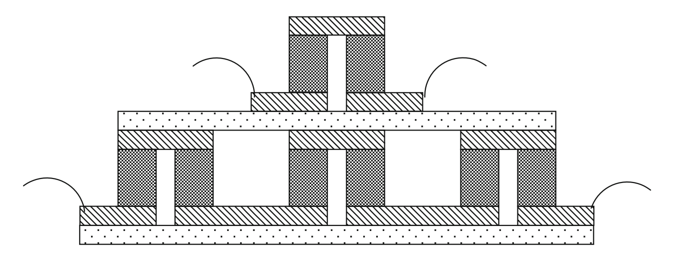
Kooi et al., J. Appl. Phys. 34, 1735 (1963)

Staging and tapering

thermoelectric

Goldsmid, "Introduction to Thermoelectricity", Springer (2009)

thermomagnetic



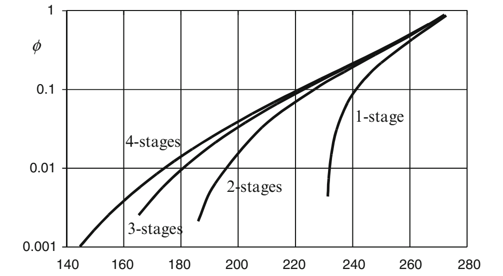
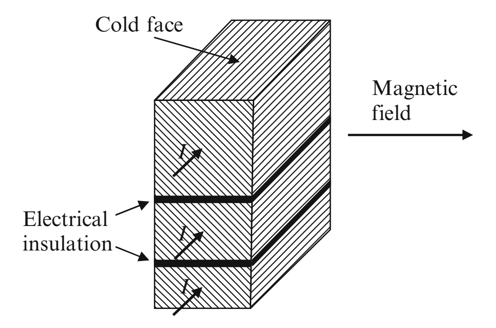
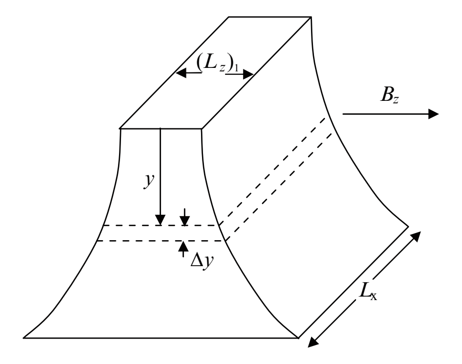
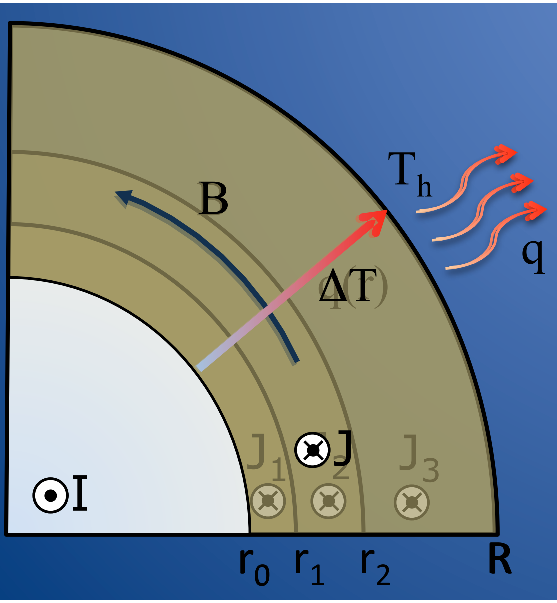


Fig. 2.8 Overall coefficient of performance plotted against heat source temperature for 1-, 2-, 3-, and 4-stage coolers. The heat sink is at 300 K and $ZT = 0.7$







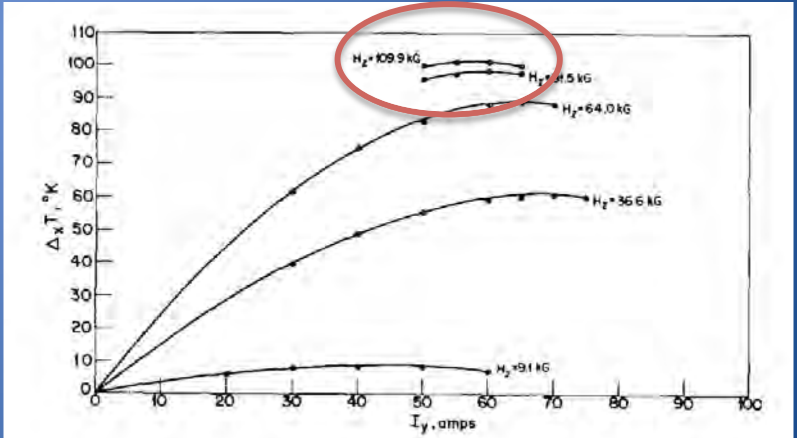
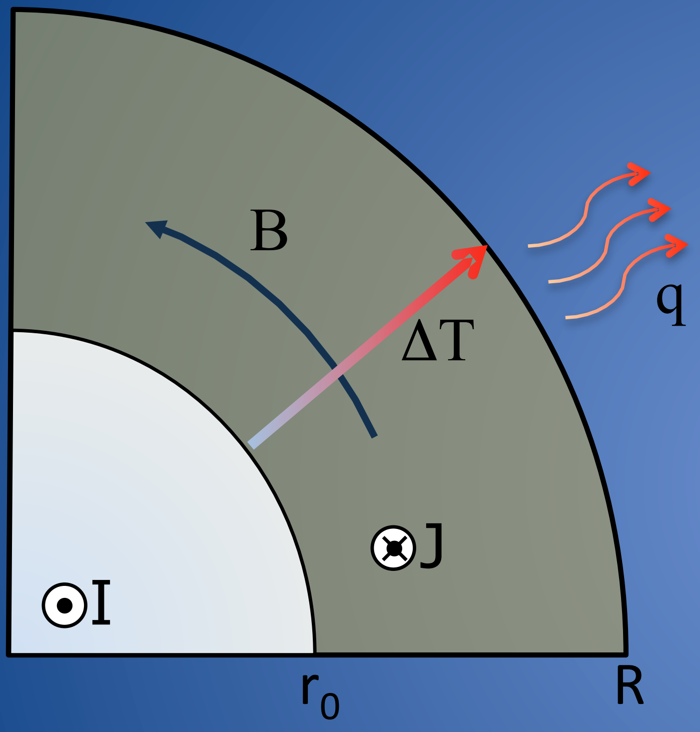


Fig. 2. Experimental curves of $\Delta_x T$ (temperature difference) vs I_y (current) for various H_z (magnetic field) for a shape ratio of 128 and a hot junction temperature of 302°K.

Harman et al., Appl. Phys. Lett. 4, 77 (1964)

Cable geometry: quantitative analysis



$$B(r) = \frac{B_0 r_0}{r} \qquad B_0 = \frac{\mu_0}{2\pi}\frac{I}{r_0}$$

All quantities constant in z
E$_z$ also constant in r

From non-equilibrium thermodynamics:

- charge (particle) current **J** and
- heat (entropy) current **q**

as a function of the generalized "forces"

- Gradient of the electrochemical potential $\nabla\mu = -\mathbf{E}$
- Gradient of temperature ∇T

Callen, "Thermodynamics, and an introduction to thermostatistics" (J. Wiley & sons (2006)

$$\begin{cases} j_z = \dfrac{E_z}{\rho} + \dfrac{NB}{\rho}\dfrac{dT}{dr} & (\mathbf{E} = -\nabla\mu) \\[2ex] q_r = \dfrac{NBT}{\rho}E_z + K(ZT-1)\dfrac{dT}{dr} & \\[2ex] \nabla\cdot\mathbf{q} = \dfrac{1}{r}\dfrac{d\ \ rq_r}{dr} = E_z j_z & \end{cases}$$

continuity equation (energy conservation)

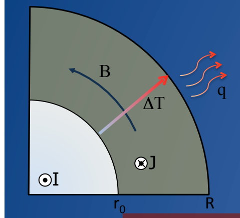
Solve for q$_r$(r) and T(r) - steady state

Analytical results (constant ρ,K,N)

Bi in high B~12T
ZT~0.35, ZaT~0.5

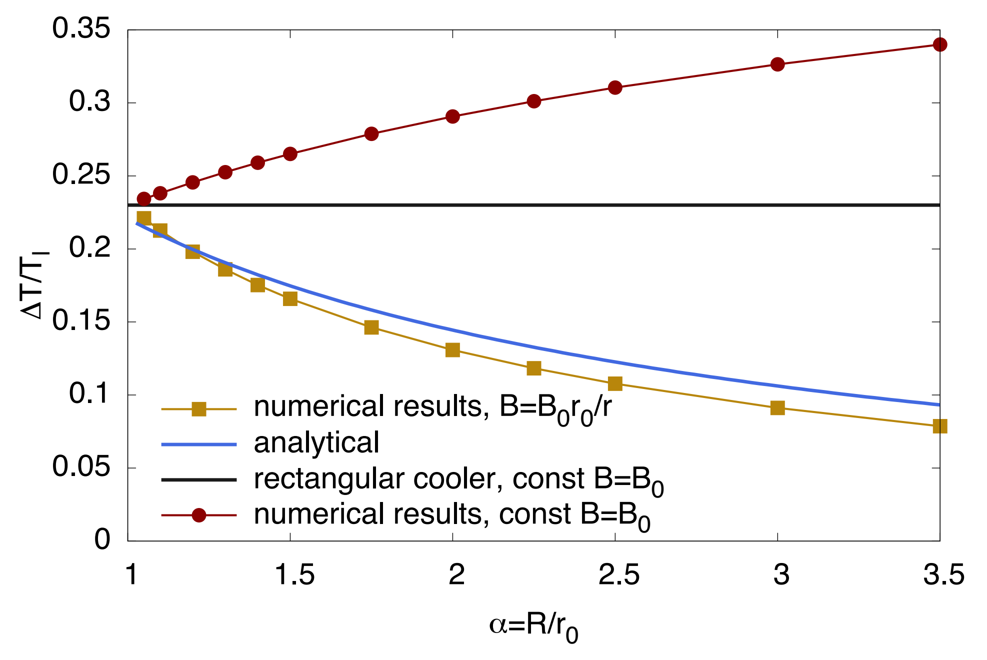
$$\Gamma_\alpha = \frac{\alpha^2-1}{2\log\alpha} - 1 \qquad \alpha = R/r_0$$

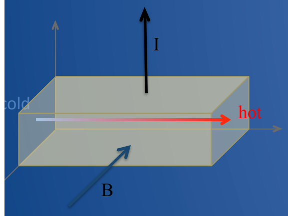
$$\Gamma_\alpha \sim \alpha - 1$$ (at small α)



$$E_z^{MAX} = \frac{N B_0 T_l}{r_0 \Gamma_\alpha}$$

$$\boxed{\Delta T_{MAX} = \frac{1}{2} Z_a^0 T_l^2 \frac{\log\alpha}{\Gamma_\alpha}}$$



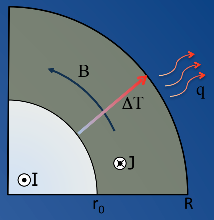


$$E_z^{MAX} = N B T_l / b$$

$$\Delta T_{MAX} = \frac{1}{2} Z T_h^2 = \frac{1}{2} Z_a(\bar{T}) T_l^2$$

Geometrical advantage superseeded by the decay of B(r) with r, but **for B~const ΔT grows with α!**

Electrical expenditure



$$\Delta T_{MAX} = \frac{1}{2} Z^0_\alpha T_l^2 \frac{\log \alpha}{\Gamma_\alpha}$$

Temperature drop

$$q_r(R) = \frac{Z^0 T_l}{R\Gamma_\alpha} K\left(\frac{T_l}{2}\frac{\alpha^2-1}{\Gamma_\alpha} + \Delta T\right)$$

Expelled heat per unit area

$$Q_{OUT} = 2\pi R q_r(R) \quad \sim \log^2 \alpha/\alpha^2$$

Expelled heat per unit cable length

The expelled heat diverges for vanishing thickness, because E_z^{MAX} diverges

$$E_z^{MAX} = \frac{N B_0 T_l}{r_0 \Gamma_\alpha}$$

$$\Gamma_\alpha \sim \alpha - 1$$

A compromise between the best DT and the expelled heat (energy spent in the cooling) has to be found!

Materials : Bismuth and alloys (e.g. Bi_xSb_{1-x}), and then?

But transport coefficients (and thus Z) do depend on Temperature and magnetic field!!

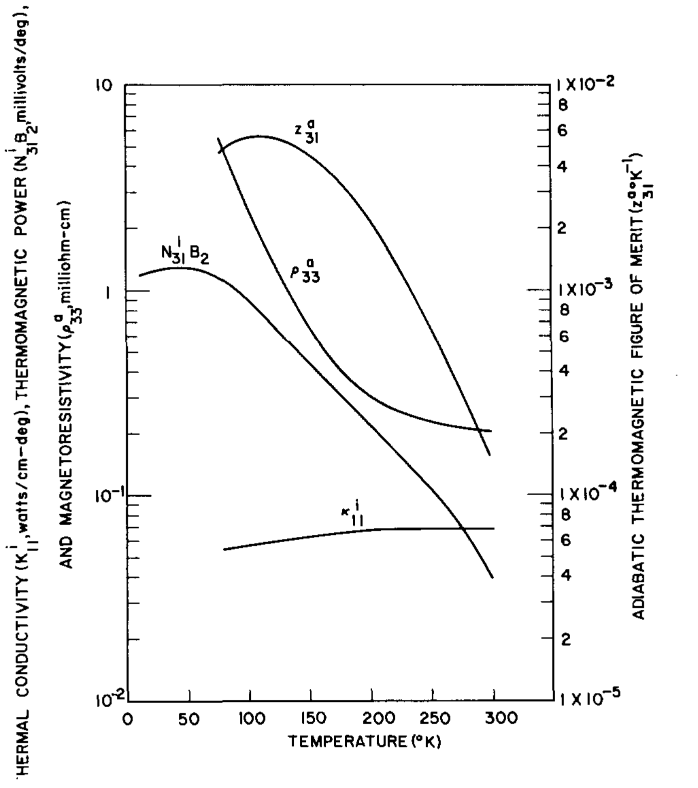


Fig. 1. The isothermal thermomagnetic power, isothermal thermal conductivity, the adiabatic resistivity, and the adiabatic thermomagnetic figure of merit of a single crystal of Bi(97)Sb(3) measured at 1 V-sec/m^2.

Cuff et al. Appl. Phys. Lett. 2, 145 (1963)

Harman et al., Sol. State El. 7, 505 (1964)

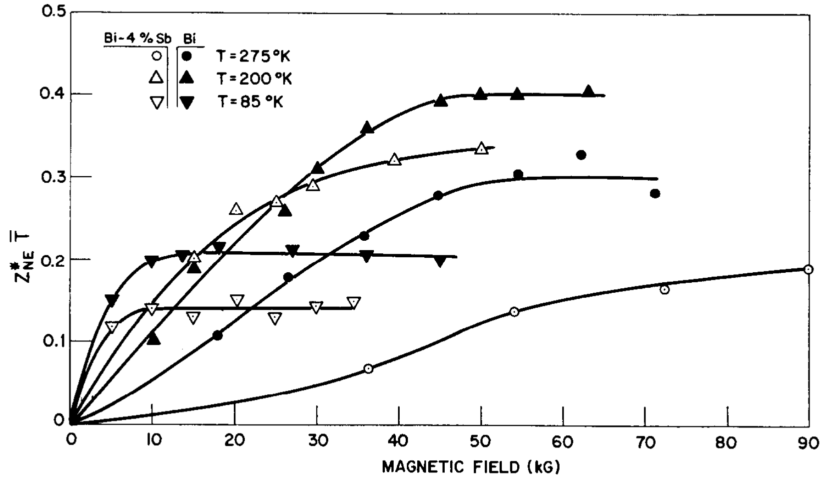
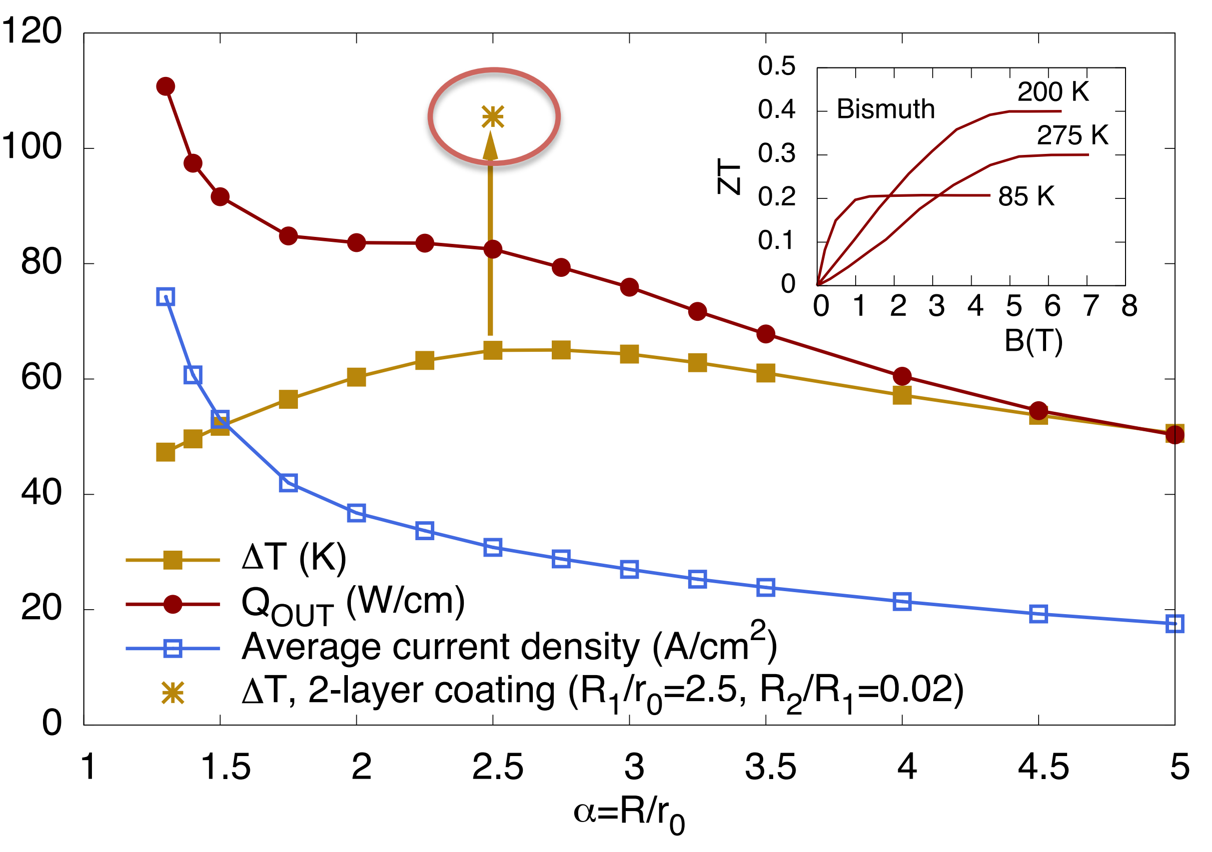


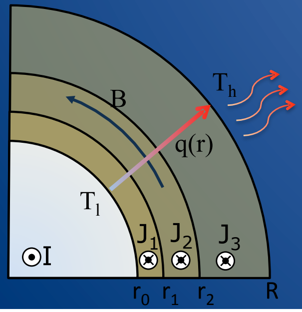
FIG. 2. Experimentally determined values of the Nernst–Ettingshausen figure of merit versus magnetic field strength for various temperatures. The values for Bi and Bi–4% Sb are represented by solid and open points, respectively.

Bismuth and alloys are the best known, but at T<100K they are known to perform less well

Best (and stable) in high magnetic fields however!

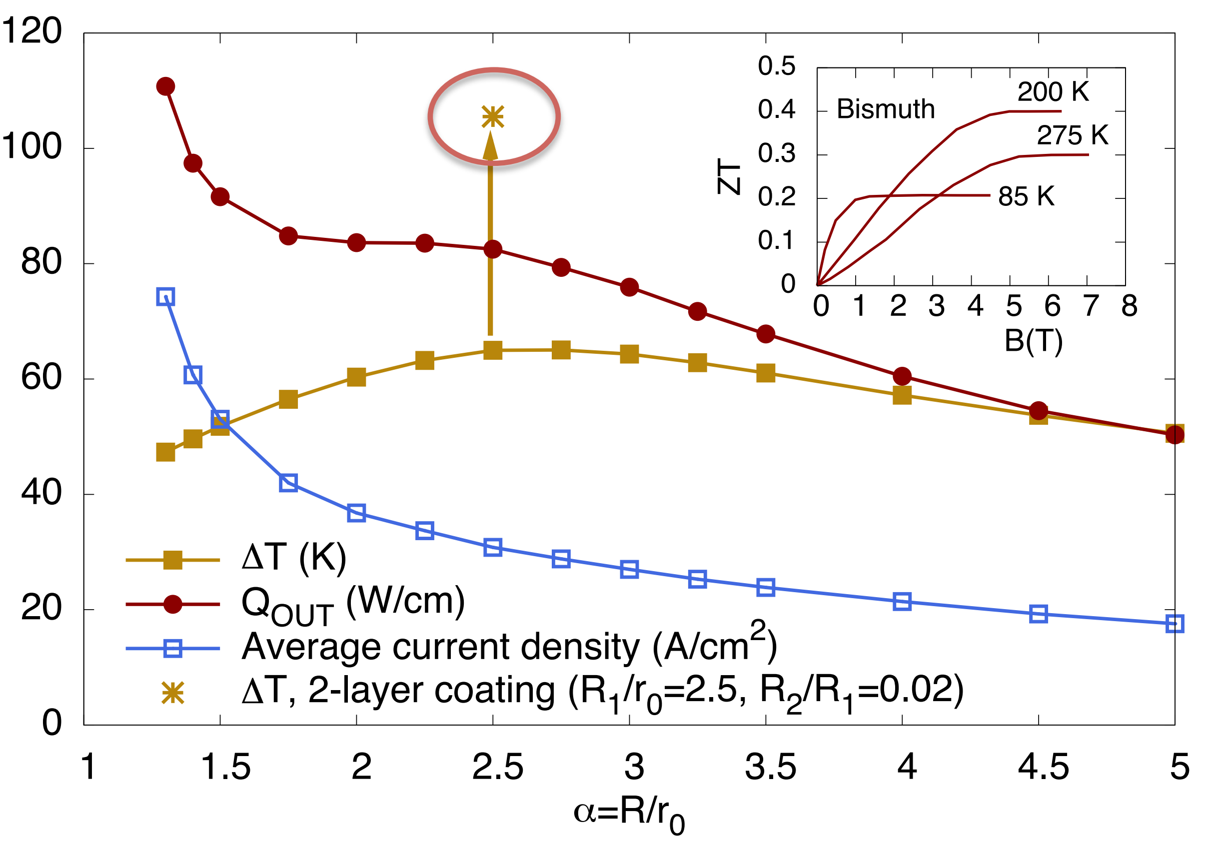
Numerical Results (Bismuth realistic parameters)

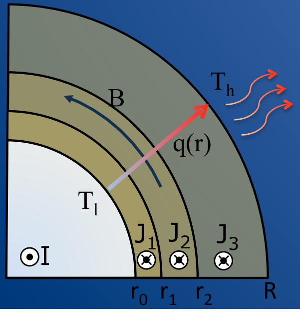




$$\Delta T_{MAX} = \frac{1}{2}\frac{Z^0}{1-\overline{ZT}}T_l^2\frac{\log\alpha}{\Gamma_\alpha} - q_{IN}\frac{r_0\log\alpha}{K(1-\overline{ZT})}$$

Numerical Results (Bismuth realistic parameters)





1 layer: ΔT~60K 2 layers: ΔT>100K !!

(however Q$_{OUT}$~1000 W/cm)

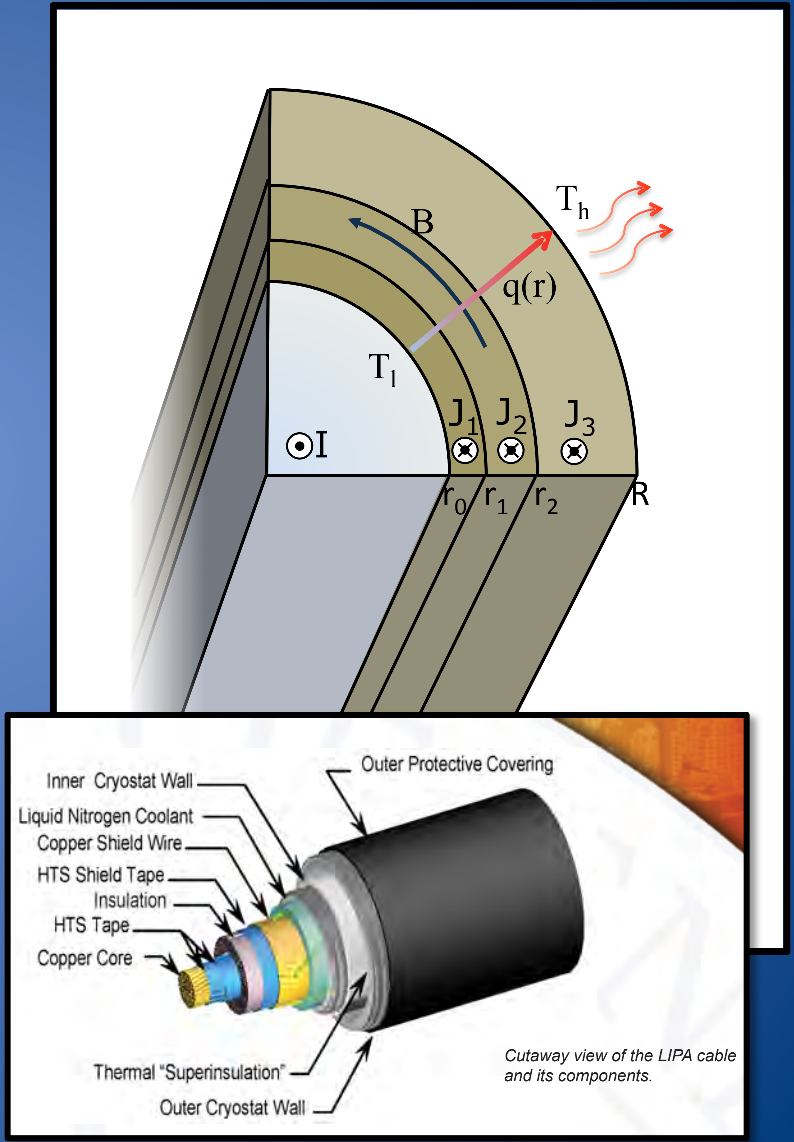
Mains questions and problems

Materials not quite there?
- More experimental data
- Improvement of materials

Metallurgy
- Properties strongly anysotropic in Bi & alloys
- insulating layer

Heat evacuation
- By 2nd principle of thermodynamics, this setup generate heats, needs evacuation

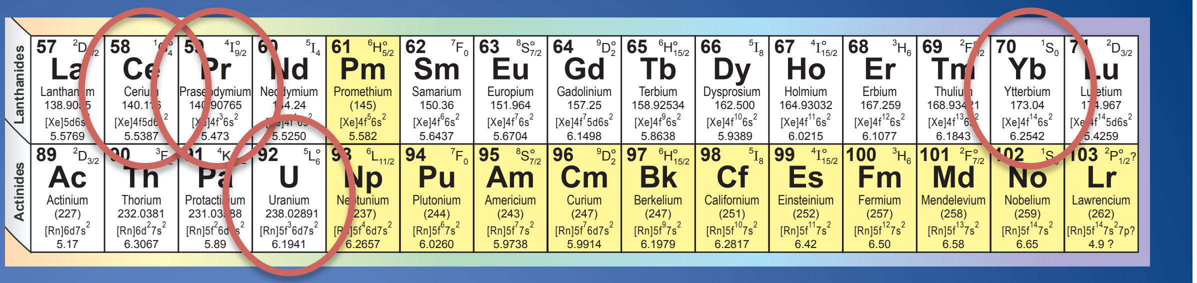
Turning on procedure?
- Normal cooling to start the SC current
- Short time-scale effects?



Cutaway view of the LIPA cable and its components.

Material optimization: heavy-fermions?

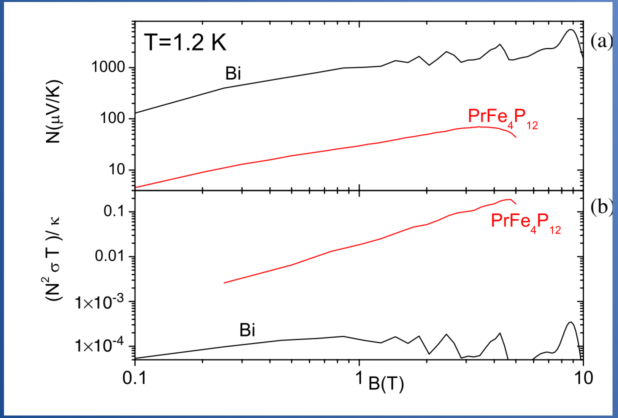
Thermoelectrics: strong seebeck found in heavy-fermions such as $CeCu_6$, $CeAl_3$, $YbAl_3$, …



… and in some Fe semiconductors (FeSb, FeSi), materials resembling "Kondo insulators"

Thermomagnetics: high Nernst coefficient in $PrFe_4P_{12}$, URu_2Si_2, …

High ZT at low temperatures!



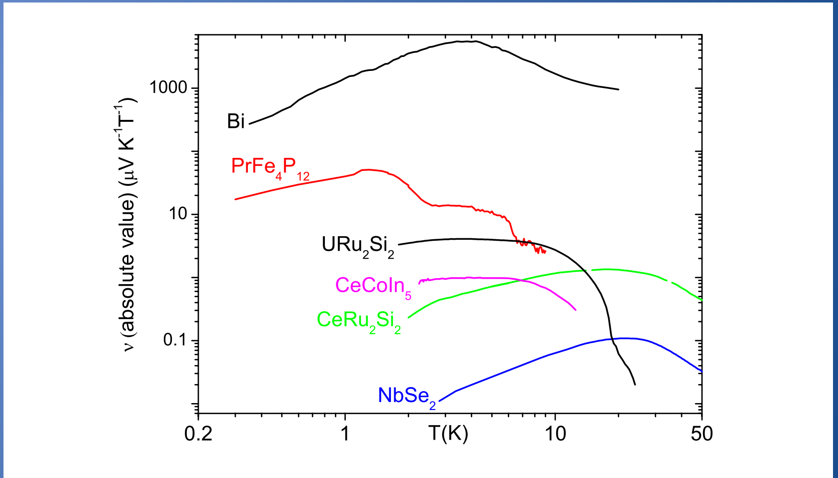
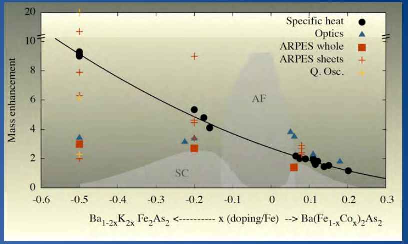


FIG. 3 (color online). The magnitude of the Nernst coefficient in bismuth compared to what is found in some other metals [4,5,7,8,12].

Behnia et al. PRL 98, 076603 (2007)

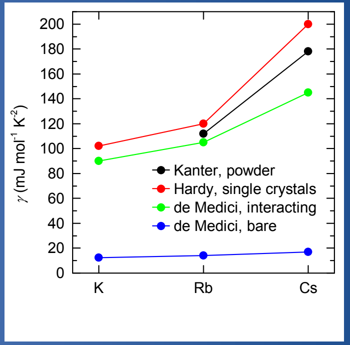
Can we improve thermoelectric/thermomagnetic performances with d-electron heavy-fermions?

Conclusions and References



- Orbital-selective Mott physics plays a key role in Fe-superconductors
- More and more supported by direct experimental evidence
- Heavy-fermionic behaviour can be found and controlled in Fe-superconductors

- LdM, G. Giovannetti and M. Capone, *Selective Mott Physics as a key to Iron superconductors*, PRL 112, 177001 (2014)
- LdM, *Weak AND strong correlations in Fe Superconductors*, in “Iron-based Superconductivity”, Springer Series in Material Sciences, Vol 211, pp 409-441 (2015) - ArXiv: 1506.01678



- Solid-state cooling for high-current cables is possible, based on Ettinshausen effect: ideal Bismuth single-crystal 1-layer: ΔT~60K, 2-layer ΔT>100K
- Improvements in thermomagnetic materials are still needed (higher ZT)
- Can we “design” new thermomagnetic materials with d-electron heavy-fermions?

LdM, *A thermomagnetic mechanism for self-cooling cables* , ArXiv:1506.01674 (2015)