Heavy Fermions and Electronic Correlations in $FeSb_2$

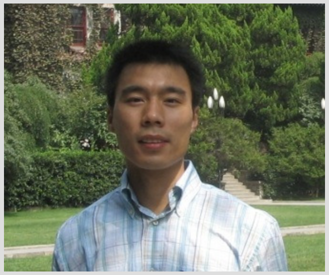
Cedomir Petrovic

Condensed Matter Physics, Brookhaven National Laboratory

Heavy Fermions and Quantum Phase Transitions, Beijing 2012

Acknowledgements

EMSC BNL



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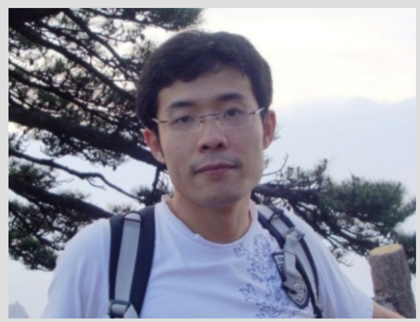
(postdoc)



Hechang Lei (雷和畅)
(postdoc)
Soon at Renmin University
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High Magnetic Field Lab
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EMSC at BNL

MAKING CRYSTALS

MEASURING CRYSTALS

ture, transport, thermodynamics, magnetization

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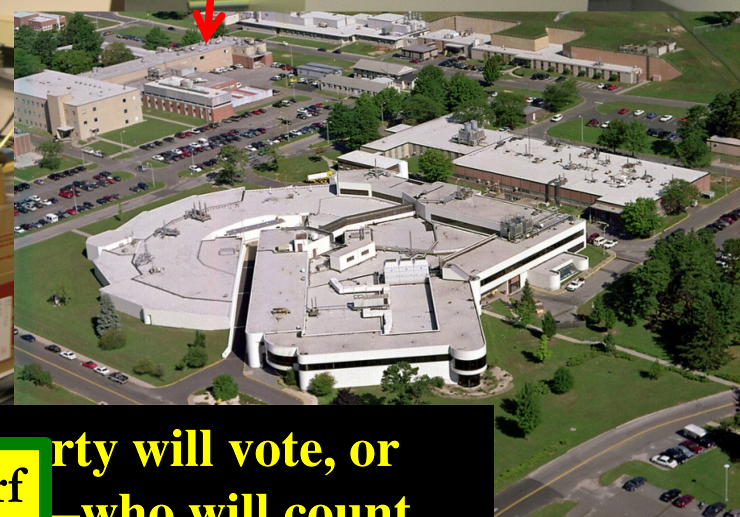


EMSC

HLD.

HELMHOLTZ ZENTRUM DRESDEN ROSSENDORF

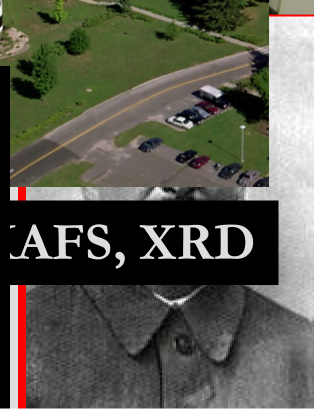
HLD Dresden Rossendorf

rty will vote, or

–who will count

iginal: Я считаю, что совершенно неважно, кто и как будет в партии голосовать; но вот что чрезвычайно важно, это - кто и как будет считать голоса).

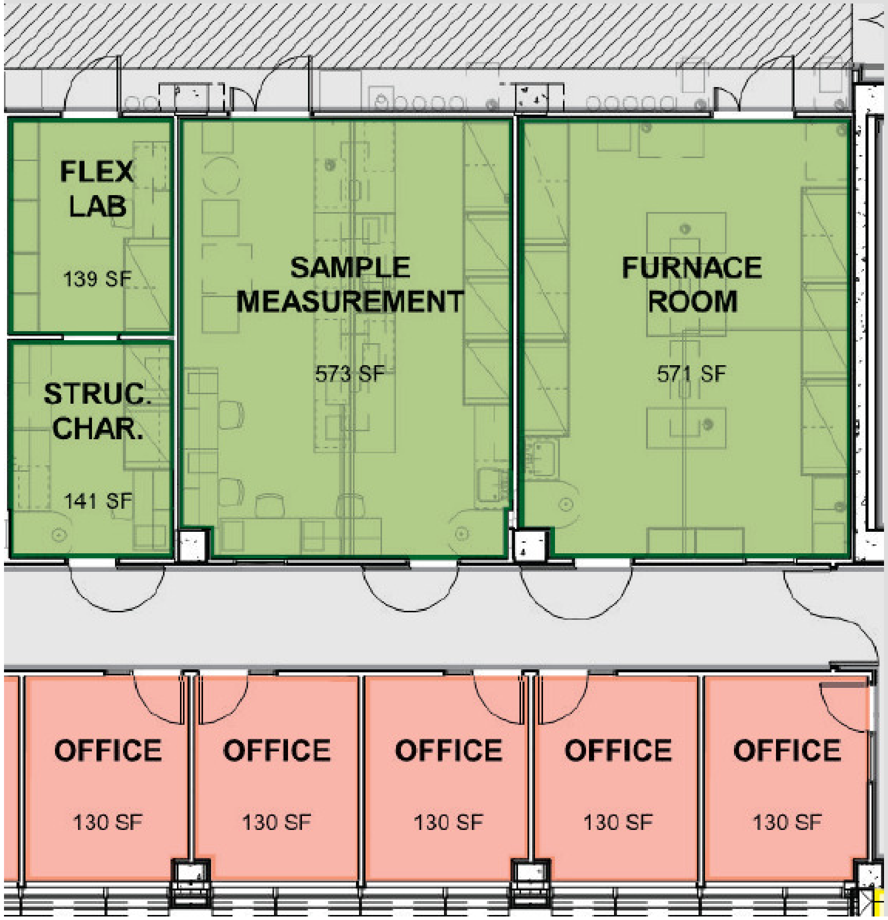
AFS, XRD



New Workplaces

ISB

- New laboratory space custom designed
- Ability to explore more materials
- Arsenides and safety?
- Lights go on in NSLS 2



NSLS2

July 2012

Mid morning, July 31.

NEW PHYSICS THROUGH NEW MATERIALS

- **Superconductivity in Fe – based Materials**
  Search for new materials. Advanced synthesis of known materials. Crystallographic phase separation. Neighboring states and materials examples.

- **Quantum Criticality**
  Advanced synthesis of known heavy fermion materials. Disorder at the QCP. Charge fluctuations at the QCP.

- **Kondo Insulator-like semiconductor with *3d* ions**
  Heavy fermions without *4f* Kondo resonance.

- **Dirac States in Bulk Crystals**
  Search for new materials. Thermoelectric properties.

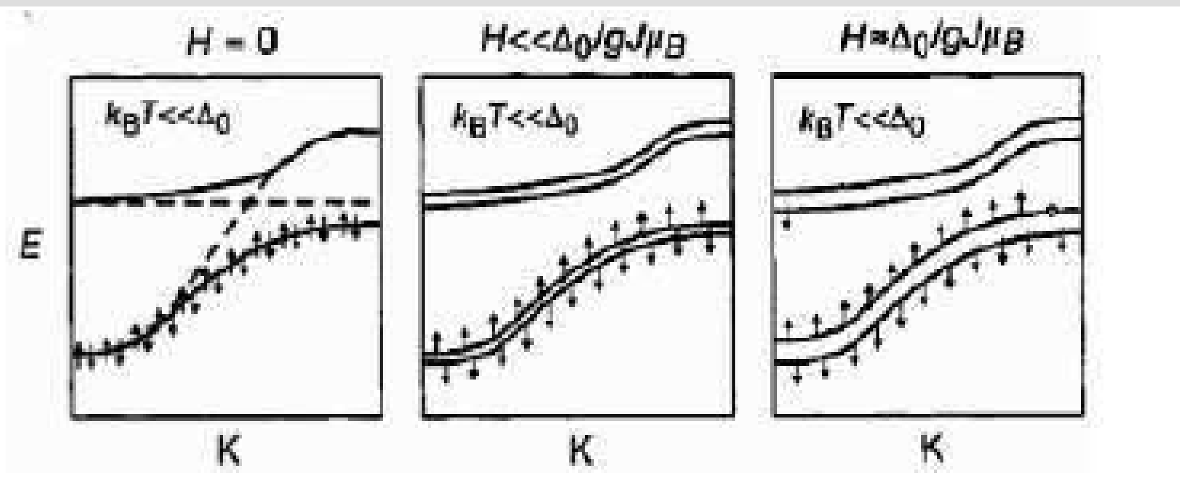
- **Materials of potential interest for Thermoelectric, Spintronic**
  Intermetallics, oxides, Mn-Ge half metallic ferromagnets.

Kondo Insulators

P. Coleman, Handbook of Magnetism and Advanced Magnetic Materials. Vol 1. John Wiley and Sons, 95-148 (2007)) ; G. Aeppli and Z. Fisk, Comments Cond. Matt. Phys. 16, 155 (1992)

High T<H: KI are local moment metals
Low T, H: Coherence in due to Kondo effect brings reduction in σ, χ_{Pauli}

Quasiparticle perspective: KI are highly renormalized "band insulators":
Gap driven by interaction effects



MIT driven by H (also doping, T)

Rare earth materials: SmB_6, $Ce_3Bi_4Pt_3$…

Single particle picture or **Many body correlations**

(A)

Single particle picture

(B)

Many body correlations

Singlet Semiconductor to Ferromagnetic Metal Transition in FeSi

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T. M. Rice
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(Received 28 September 1995)

Adding the local Coulomb repulsion to the local density approximation, the so-called LDA + U scheme, leads us to predict a first order transition from a singlet semiconductor to ferromagnetic metal in FeSi with increasing magnetic field. Extensions to finite temperature lead to the interpretation that the anomalous behavior at room temperature and zero field arises from proximity to the critical point of this transition. This critical point at a finite field may be accessible in currently available magnetic fields.

PACS numbers: 75.30.Kz, 71.30.+h, 75.10.Lp

FeSi displays an unusual crossover from a singlet semiconducting ground state with a narrow band gap to a metal with an enhanced spin susceptibility and a Curie-Weiss temperature dependence in the vicinity of room temperature [1]. Various models have been put forward to explain this behavior, starting with the very narrow band description of Jaccarino *et al.* [2]. Takahashi and Moriya [3] proposed a nearly ferromagnetic semiconductor model, predicting thermally induced spin fluctuations which were subsequently confirmed experimentally [4]. Recently, models based on treating FeSi as a transition metal analog of the Kondo insulators found in heavy-fermion–rare-earth systems have been much discussed [5,6].

Electronic structure calculations using a local density approximation (LDA) by Mattheiss and Hamann [7] correctly account for the narrow gap semiconducting ground state but more is required to explain the anomalous behavior. In this Letter we report calculations based on the LDA + U scheme, a generalization of the LDA method introduced by Anisimov *et al.* [8,9] to include the influence of local Coulomb interactions on the electronic structure and magnetic properties of real systems in the

$n_{m\sigma}$ is the occupancy of a particular $d_{m\sigma}$ orbital

$$E_{av} = \tfrac{1}{2}UN(N-1) - \frac{1}{4}JN(N-2). \qquad (1)$$

But LDA does not properly describe the full Coulomb and exchange interactions between d electrons in the same d shell. So Anisimov *et al.* [8,9] suggested to subtract E_{av} from the LDA total energy functional and to add orbital- and spin-dependent contributions to obtain the exact (in the mean-field approximation) formula

$$E = E_{LDA} - E_{av} + \frac{1}{2}\sum_{m,m',\sigma} U_{mm'} n_{m\sigma} n_{m'-\sigma} + \frac{1}{2}\sum_{m\neq m',m',\sigma} (U_{mm'} - J_{mm'}) n_{m\sigma} n_{m'\sigma}. \qquad (2)$$

Taking the derivative with respect to $n_{m\sigma}$ gives the orbital-dependent one-electron potential

$$V_{m\sigma}(\vec{r}) = V_{LDA}(\vec{r}) + \sum_{m'} (U_{mm'} - U_{eff}) n_{m'-\sigma} + \sum_{m'\neq m} (U_{mm'} - J_{mm'} - U_{eff}) n_{m\sigma}$$

VOLUME 71, NUMBER 11 PHYSICAL REVIEW LETTERS 13 SEPTEMBER 1993

Unconventional Charge Gap Fo

application of this to PAM, Hubbard where only few bands are important

Z. Schlesinger

ights, New York

Z. Fisk, Hai-Tao Zhang, and M. B. Maple

$$\int_0^\infty \sigma(\omega)d\omega = \frac{ne^2}{m}$$

for all electrons in all bands

$$\int_0^\omega \sigma(\omega)d\omega = \frac{\pi}{V}\,\mathrm{Im}\langle[P,J]\rangle \sim \varepsilon_K \sim m^*$$

PHYSICAL REVIEW B VOLUME 54, NUMBER 12 15 SEPTEMBER 1996-II

Transfer of spectral weight in spectroscopies of correlated electron systems

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VOLUME 72, NUMBER 4 PHYSICAL REVIEW LETTERS 24 JANUARY 1994

Kondo Coupling Induced Charge Gap in $Ce_3Bi_4Pt_3$

B. Bucher and Z. Schlesinger

IBM T.J. Watson Research Center, Yorktown Heights, New York 10958

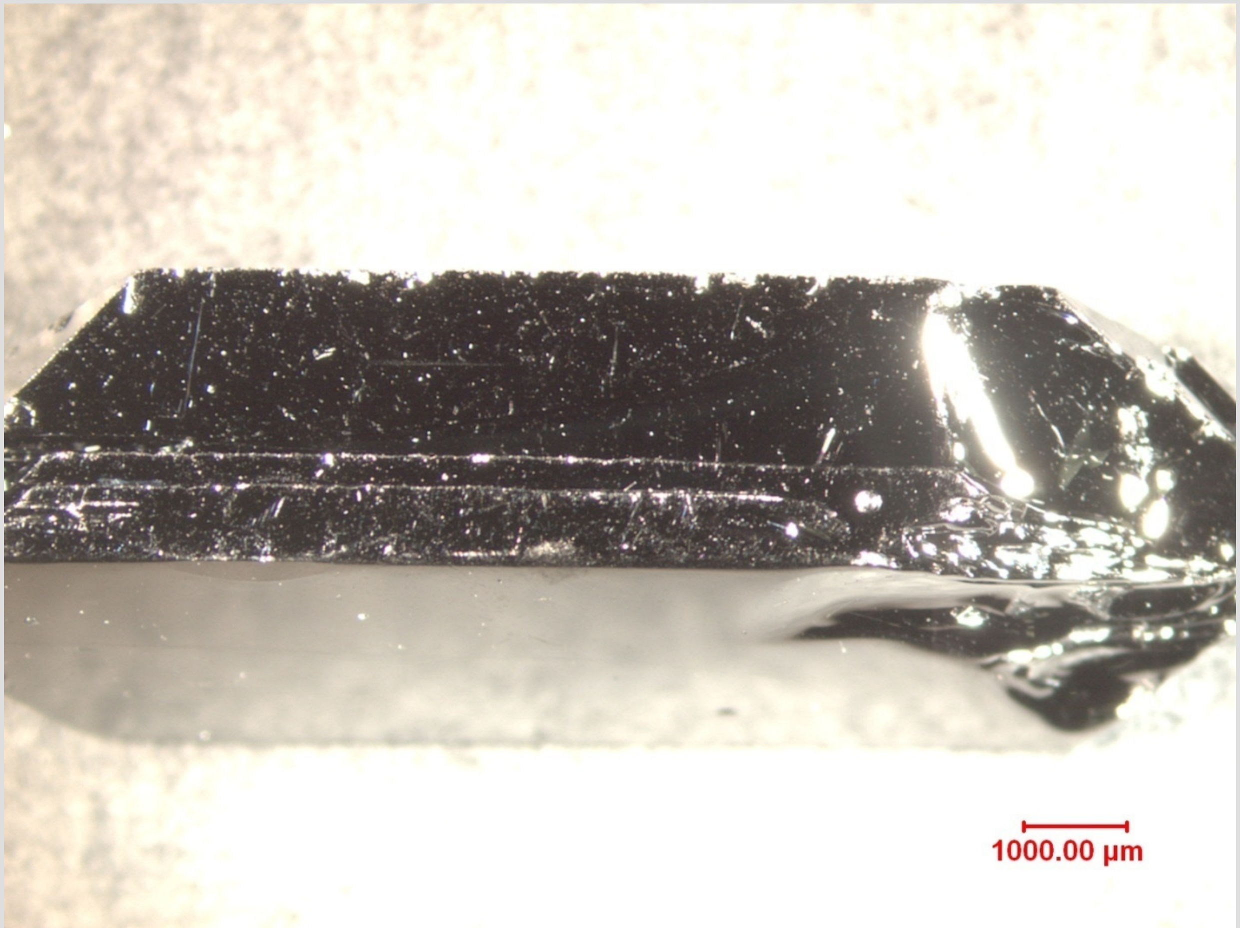
P. C. Canfield and Z. Fisk

Los Alamos National Laboratory, Los Alamos, New Mexico 87545

(Received 18 August 1993)

Measurements of the infrared reflectivity of the Kondo insulator $Ce_3Bi_4Pt_3$ as reported. Near room temperature the charge dynamics are comparable to those of a heavy fermion compound in the incoherent regime; however, below 100 K the depletion of the low frequency conductivity signifies the development of a charge gap at low frequency ($\sim$300 cm^{-1}). The temperature dependence of the depleted spectral weight scales with the quenching of the Ce 4f moments, demonstrating that the gap formation is due to the local Kondo coupling of charge carriers to the Ce magnetic moments. The spectral weight which disappears as the gap forms must be displaced to energies much larger than the gap.

New Model Material: $FeSb_2$

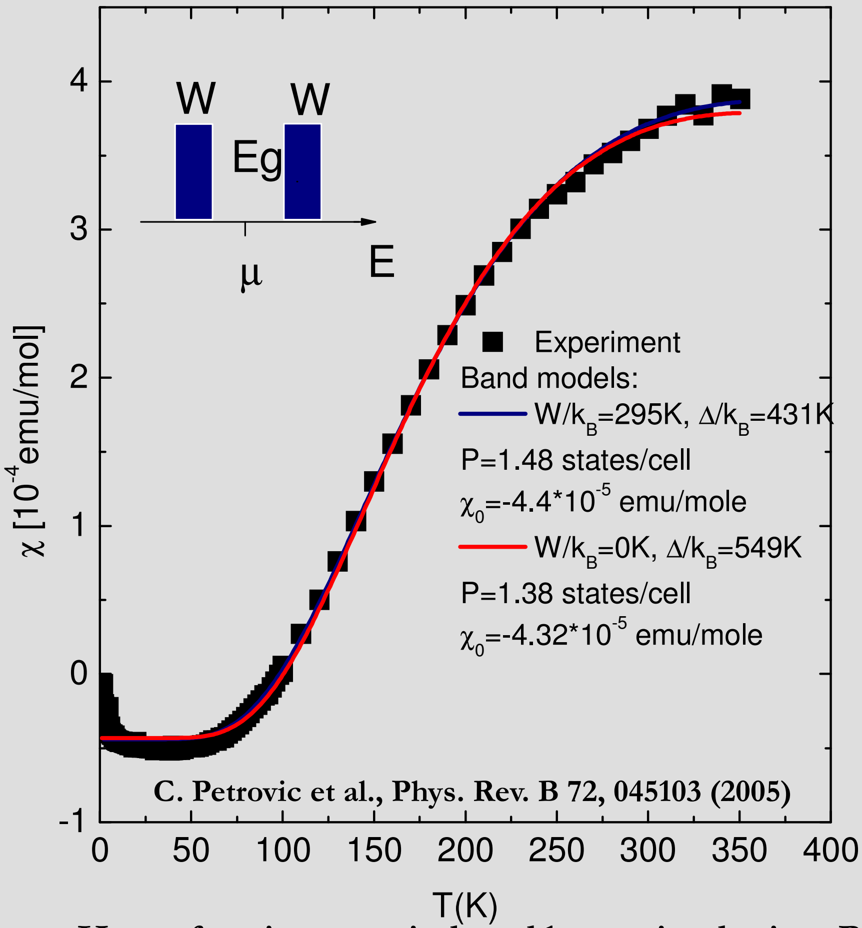


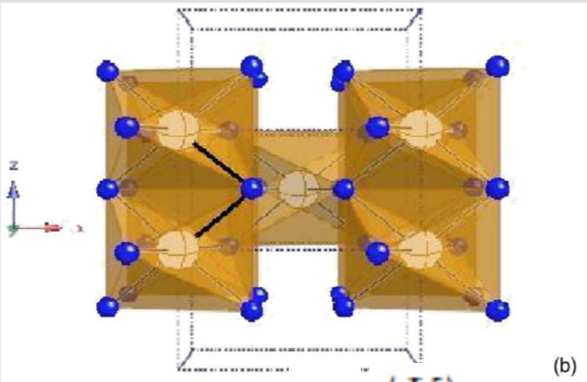
Correlated Electron (Kondo) Semiconductors

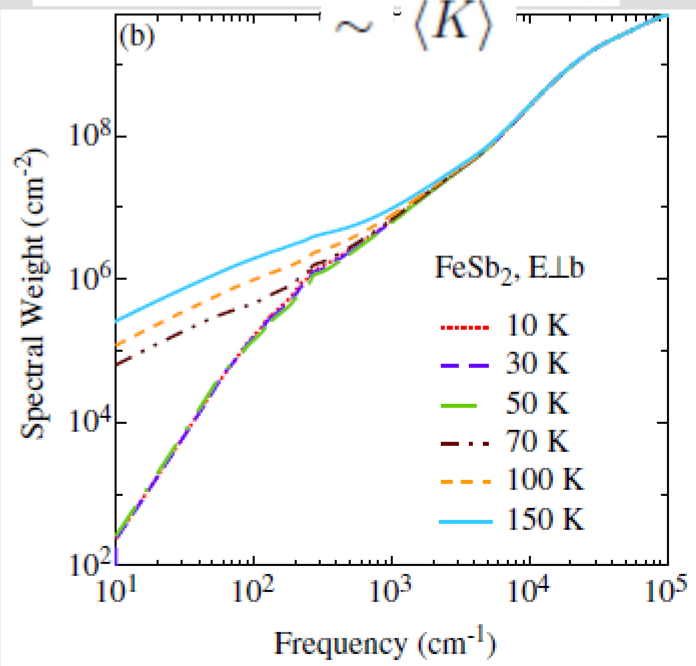
CeNiSn, CeRhSb: nodal KI – hybridization vanishes along certain directions

What about 3d electron "relatives" of Kondo Insulators?

$$\chi(T) = -2\mu_B^2 \int_{c-band} N(E)\frac{\partial f(E,\mu,T)}{\partial E}dE$$



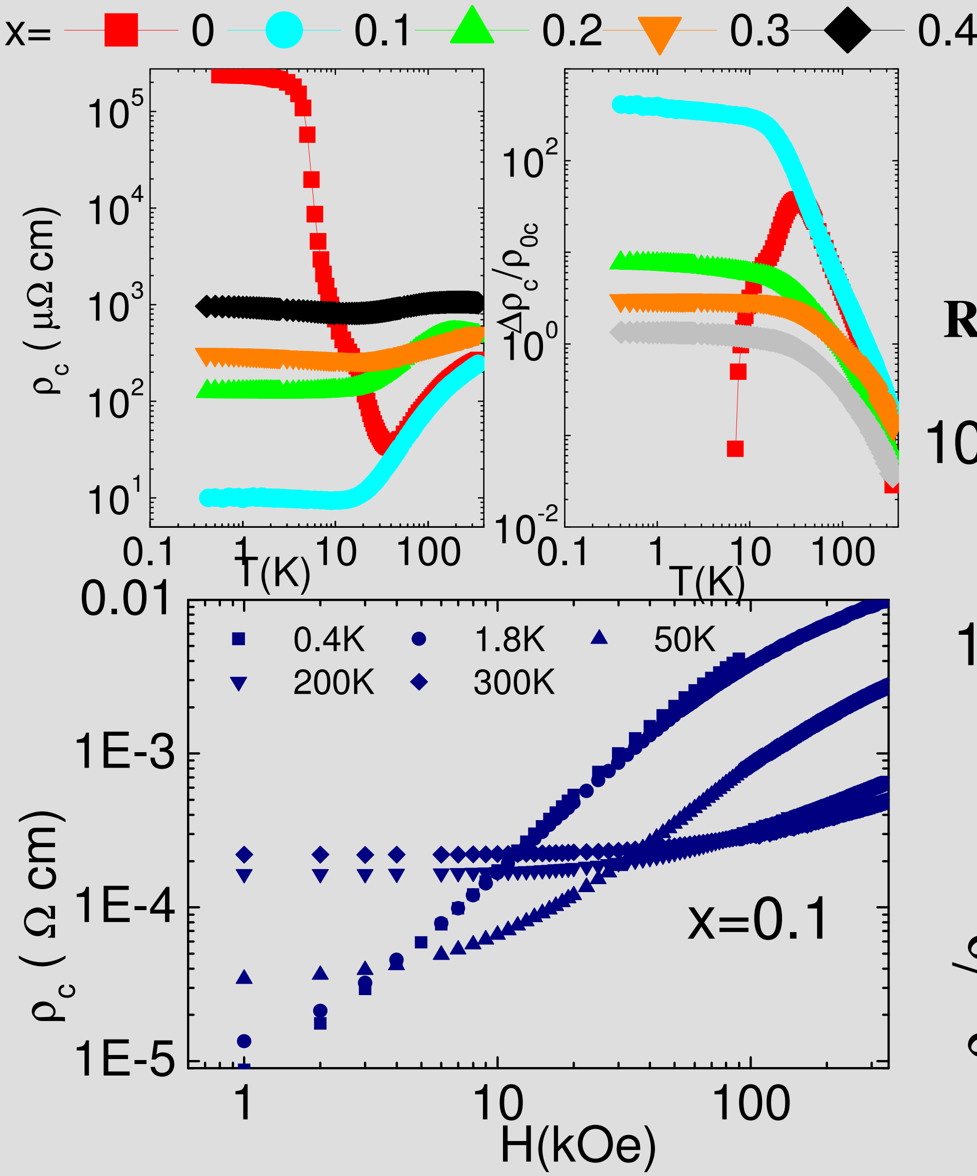




Gap recovery in eV range in $FeSb_2$
Eur. Phys. J. B 54, 175 (2006)

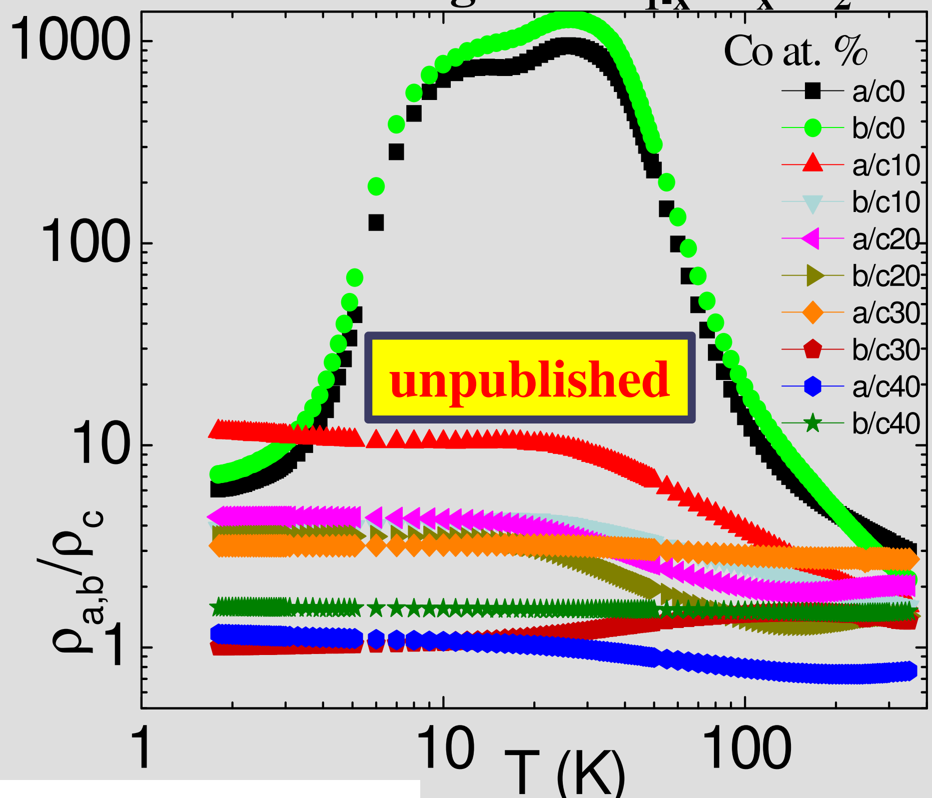
Heavy fermion state induced by carrier doping: Phys. Rev. B 74, 205105 (2006), Phys. Rev. B 74, 195130 (2006)

Colossal Magnetoresistance



$Fe_{1-x}Co_xSb_2$

Reduction of quasi 1-D character of ρ(T) with increasing x in $Fe_{1-x}Co_xSb_2$



Rongwei Hu (胡荣伟) et al, Phys. Rev. B 77, 085212 (2008)

Hall Constant

Rongwei Hu (胡荣伟) et al, Phys. Rev. B 77, 085212 (2008)

- ~~Magnetic moments: $\rho_{xy}(H)=R_0H+R_sM(H)$~~
- Two band model

$$\alpha_2 = f_1\mu_1 + f_2\mu_2$$
$$\beta_2 = (f_1\mu_2 + f_2\mu_1)\mu_1\mu_2$$
$$\beta_3 = (f_1\mu_2 + f_2\mu_1)^2$$

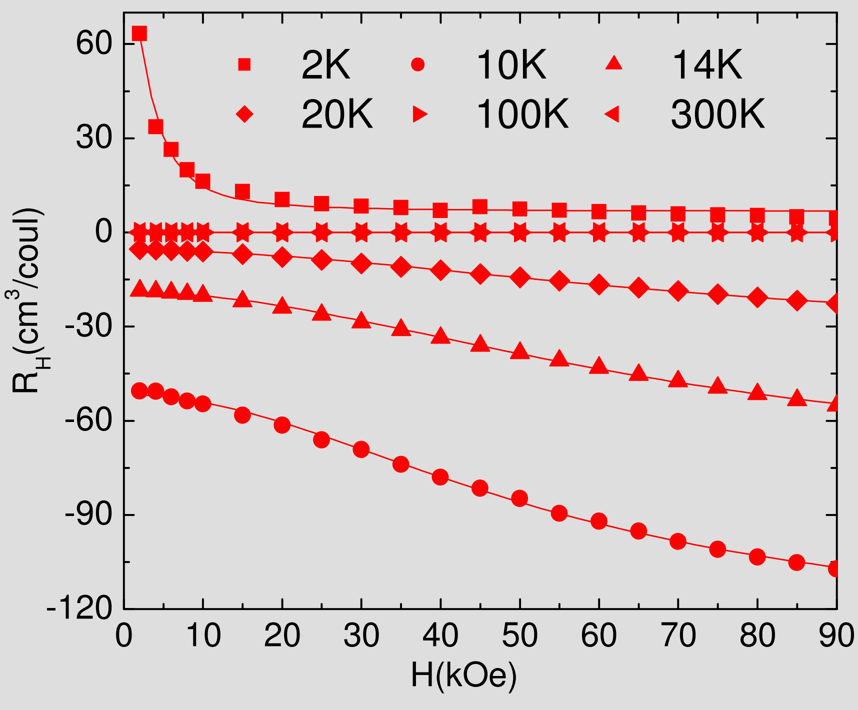
Hall Constant:

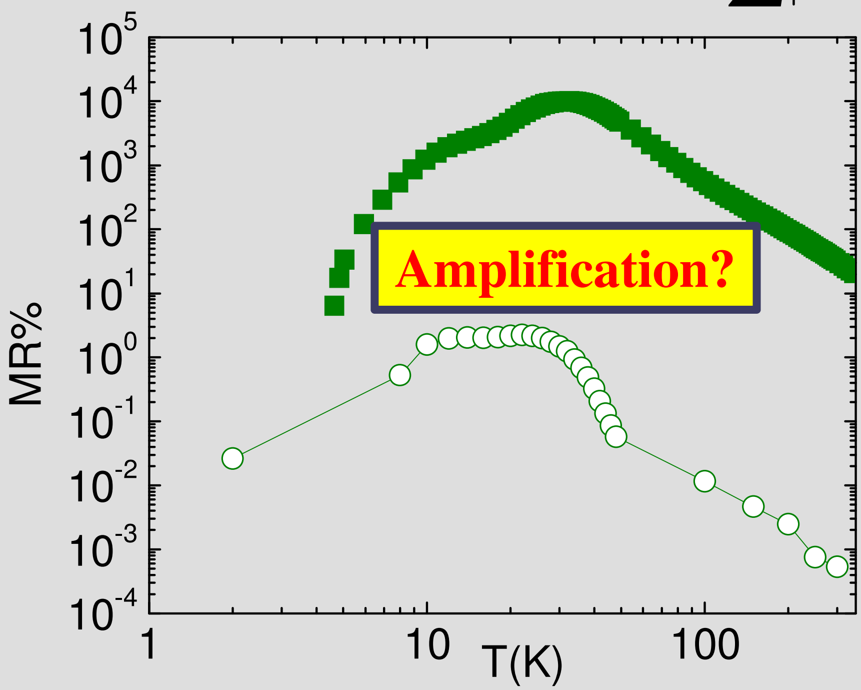
$$R_H = \frac{\rho_{xy}}{H} = \rho_0 \frac{\alpha_2 + \beta_2 H^2}{1+\beta_3 H^2}$$

Magnetoresistance:

$$MR = \frac{f_1 f_2 (\mu_1 - \mu_2)^2 H^2}{1+\beta_3 H^2}$$

$$\rho_0 = \rho(B=0);\ f_i = \frac{n_i\mu_i}{\sum |n_i\mu_i|}$$





MR in $Fe_{1-x}Co_xSi$

Magnetoresistance from quantum interference effects in ferromagnets

N. Manyala*, Y. Sidis*†, J. F. DiTusa*, G. Aeppli‡, D.P. Young§ & Z. Fisk§

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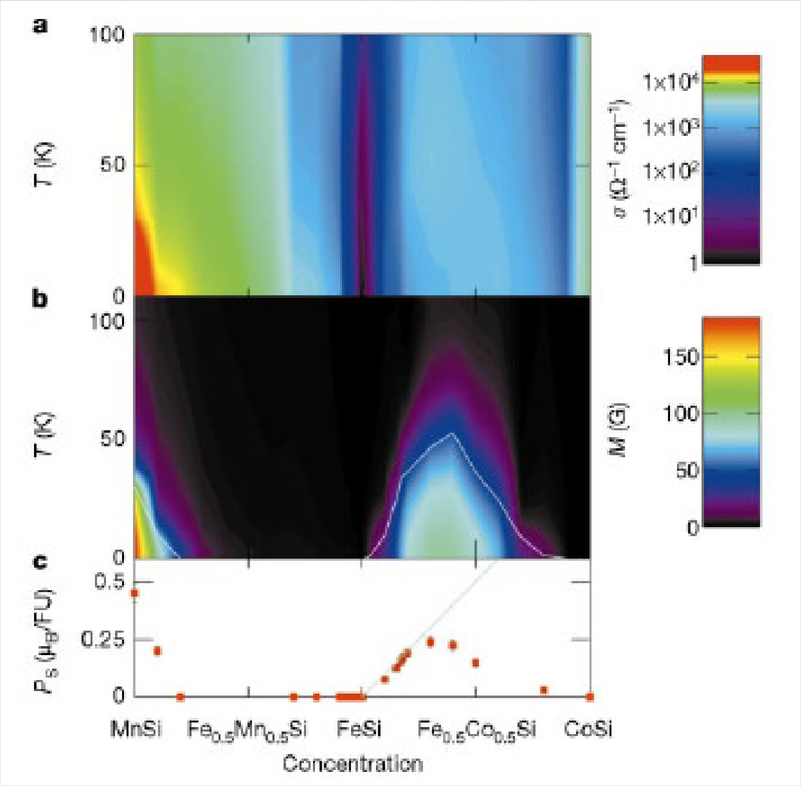
§ *National High Magnetic Field Facility, Florida State University, Tallahassee, Florida 32306, USA*

The desire to maximize the sensitivity of read/write heads (and thus the information density) of magnetic storage devices has stimulated interest in the discovery and design of new magnetic materials exhibiting magnetoresistance. Recent discoveries include the 'colossal' magnetoresistance in the manganites[1–4] and the enhanced magnetoresistance in low-carrier-density ferromagnets[4–6]. An important feature of these systems is that the electrons involved in electrical conduction are different from those responsible for the magnetism. The latter are localized and act as scattering sites for the mobile electrons, and it is the field tuning of the scattering strength that ultimately gives rise to the observed magnetoresistance. Here we argue that magnetoresistance can arise by a different mechanism in certain ferromagnets—quantum interference effects rather than simple scattering. The ferromagnets in question are disordered, low-carrier-density magnets where the same electrons are responsible for both the magnetic properties and electrical conduction. The resulting magnetoresistance is positive (that is, the resistance increases in response to an applied magnetic
weakly temperature-dependent below the Curie



Nature 404, 581 (2000)

Magnetoresistance from quantum interference effects in ferromagnets

N. Manyala*, Y. Sidis*†, J. F. DiTusa*, G. Aeppli‡, D.P. Young§ & Z. Fisk§

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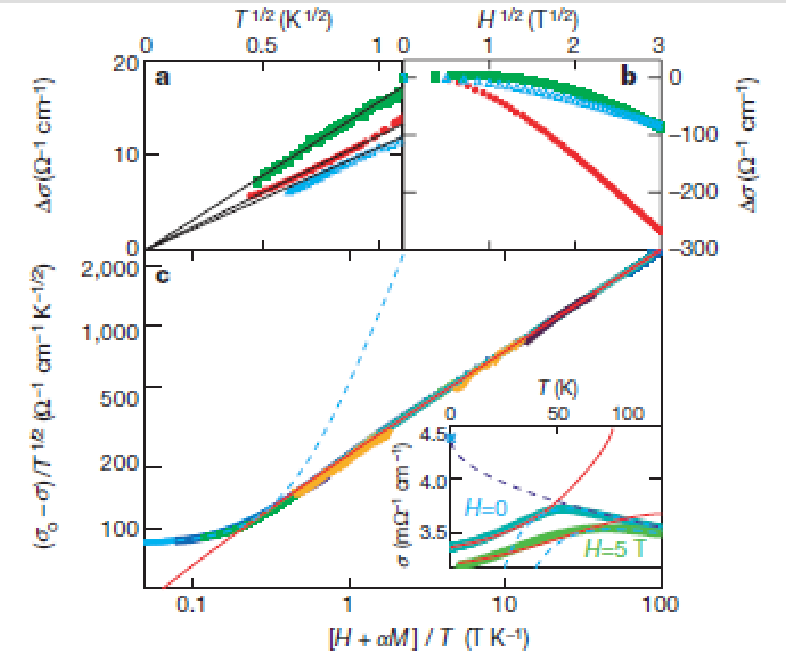
MR in $Fe_{1-x}Co_xSi$



The standard theory for paramagnetic disordered metals usefully encapsulates $\sigma(H, T)$ by $(\sigma - \sigma_0)/T^{1/2} = f(g\mu_B H/k_B T)$ where $f(x)$ is a scaling function whose limiting form is x^2 for $x \ll 1$ and $x^{1/2}$ for $x \gg 1$ (refs 24 and 25). Because $Fe_{1-y}Co_ySi$ is, to our knowledge, the first ordered ferromagnet for which the $T^{1/2}$ and $H^{1/2}$ terms are present, no theory is available for ferromagnets. Even so, it seems reasonable to believe that the main difference between paramagnets and ferromagnets is simply that for the ferromagnet, in addition to the external field, there is a large spontaneous field due to the ordered moment. Thus, the effective field is really $H_{eff} = H + \alpha M$ (where α is a constant) rather than H alone. We then imagine that for the ferromagnet, we should simply insert H_{eff} where H appears in the expressions for $\sigma(H, T)$ derived for disordered paramagnets with electron–electron interactions[27].

Nature 404, 581 (2000)

MR in $Fe_{1-x}Co_xSi$

PHYSICAL REVIEW B **72**, 224431 (2005)

Doping dependence of transport properties in $Fe_{1-x}Co_xSi$

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[1]*Spin Superstructure Project, ERATO, Japan Science and Technology Agency (JST), Tsukuba 305-8562, Japan*

[2]*Correlated Electron Research Center (CERC), National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba 305-8562, Japan*

[3]*Department of Advanced Materials Science, University of Tokyo, Kashiwa 277-8581, Japan*

[4]*Department of Applied Physics, University of Tokyo, Tokyo 113-8656, Japan*

(Received 7 July 2005; revised manuscript received 27 September 2005; published 23 December 2005)

The positive magnetoresistance has been investigated for $Fe_{1-x}Co_xSi$ single crystals in a wide range of doping ($0.05 \lesssim x \lesssim 0.7$). Most of the magnetoconductivity data are found to scale well with the magnetization. This is inconsistent with the quantum interference scenario proposed by Manyala *et al.* [Nature **404**, 581 (2000)]. We have shown that the decrease of density of the minority spin band with high mobility in the course of Zeeman splitting is relevant to the positive magnetoresistance. The nearly half-metallic nature in this system seems to enhance the magnetoresistance. The pressure dependence of resistivity has been measured for $Fe_{0.7}Co_{0.3}Si$. T-linear behavior has been found in the resistivity above 7 GPa, where the helical spin order is completely suppressed. This temperature dependence reproduces that of the hypothetical resistivity of the nonmagnetic state deduced by the analysis of the magnetoresistance. We have investigated the large Hall conductivity in $Fe_{1-x}Co_xSi$ ($\sim 40\ \Omega^{-1}\ \mathrm{cm}^{-1}$ at a maximum). The doping dependence of the Hall conductivity is almost parallel with those of the critical field and the wave vector of the helical spin state. This suggests that the Hall conductivity is proportional to the effective spin-orbit interaction. We have also observed the doping dependence of the Seebeck coefficient for $Fe_{1-x}Co_xSi$. In the underdoped region ($x \lesssim 0.1$), the negative Seebeck coefficient is enhanced at low temperature below 100 K, corresponding to the steep doping variation of the resistivity in this temperature region. In the higher doping region ($x \gtrsim 0.2$), the Seebeck coefficient shows a gradual upturn at low temperatures ($\lesssim 100$ K). This is caused by the electronic structural change occurring with the transition from the paramagnetic to the ferromagnetic state.

Direct Analog of FeSi

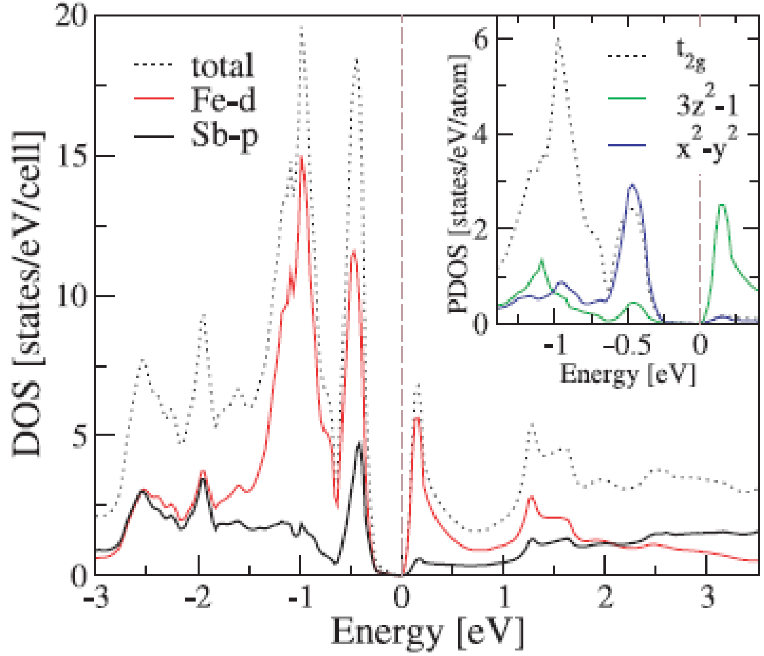


Fig. 1. Total and partial densities of states for $FeSb_2$ from the LDA calculation. Inset shows partial t_{2g}-DOS and $3z^2 - r^2$, $x^2 - y^2$ orbitals DOS of Fe-3d states. The Fermi energy corresponds to zero.

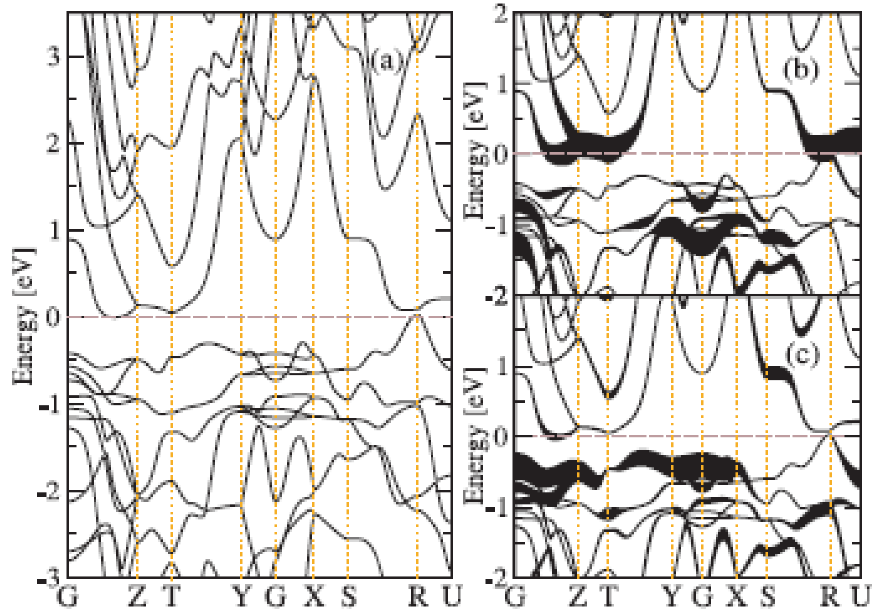


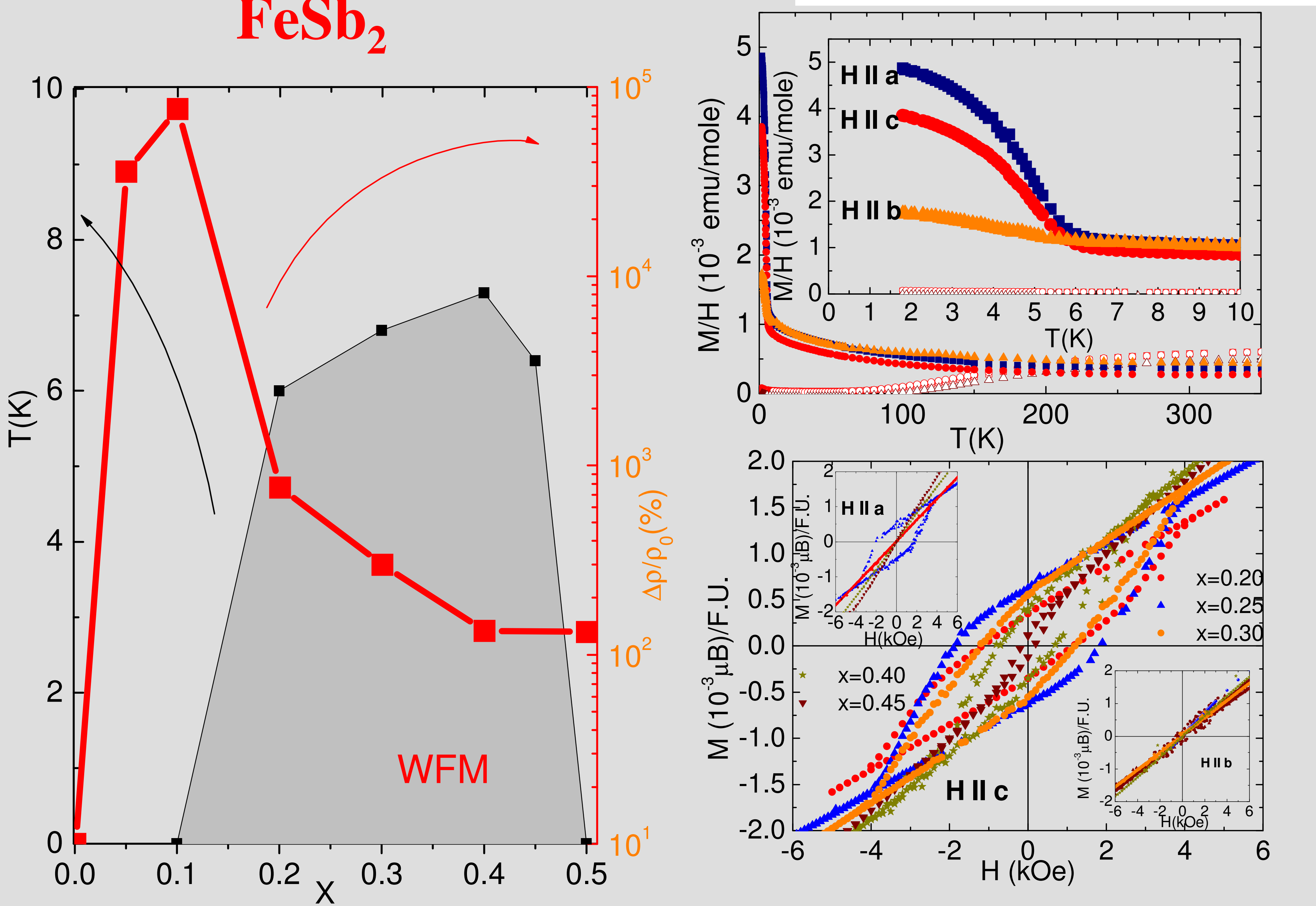
Fig. 2. (a) Band structure of $FeSb_2$ from the LDA calculation. Right panels show partial contributions of (b) $3z^2 - r^2$ and (c) $x^2 - y^2$ orbitals to the total band structure. Additional broadening of the bands corresponds to the contribution of the orbital. The Fermi energy corresponds to zero.

A. V. Lukoyanov, V. V. Mazurenko, V. I. Anisimov, M. Sigrist and T. M. Rice, Eur. Phys. J. B 53, 207 (2006)

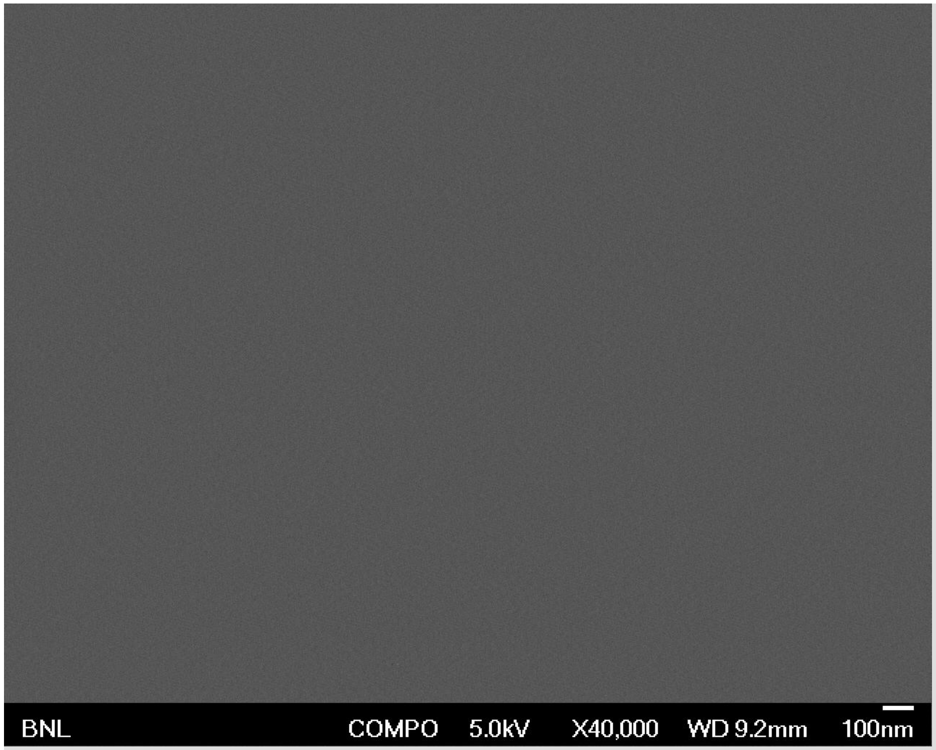
We have applied the LDA+U method to $FeSb_2$. As in the case of FeSi a second local minimum appears in the energy vs. uniform magnetization at a value of 1 μ_B per Fe (see Fig. 3). In this set of calculations we performed fixed spin moment procedure [3]. Again the exact energy

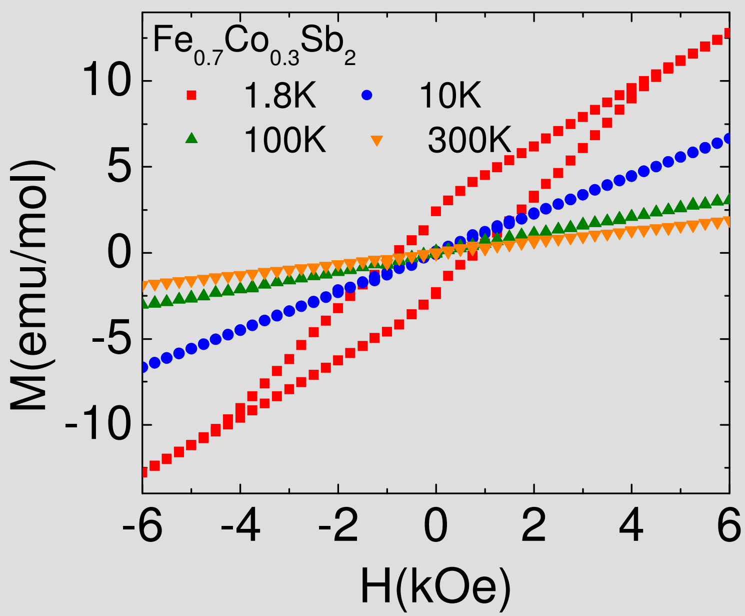
Weak Ferromagnetism in $FeSb_2$

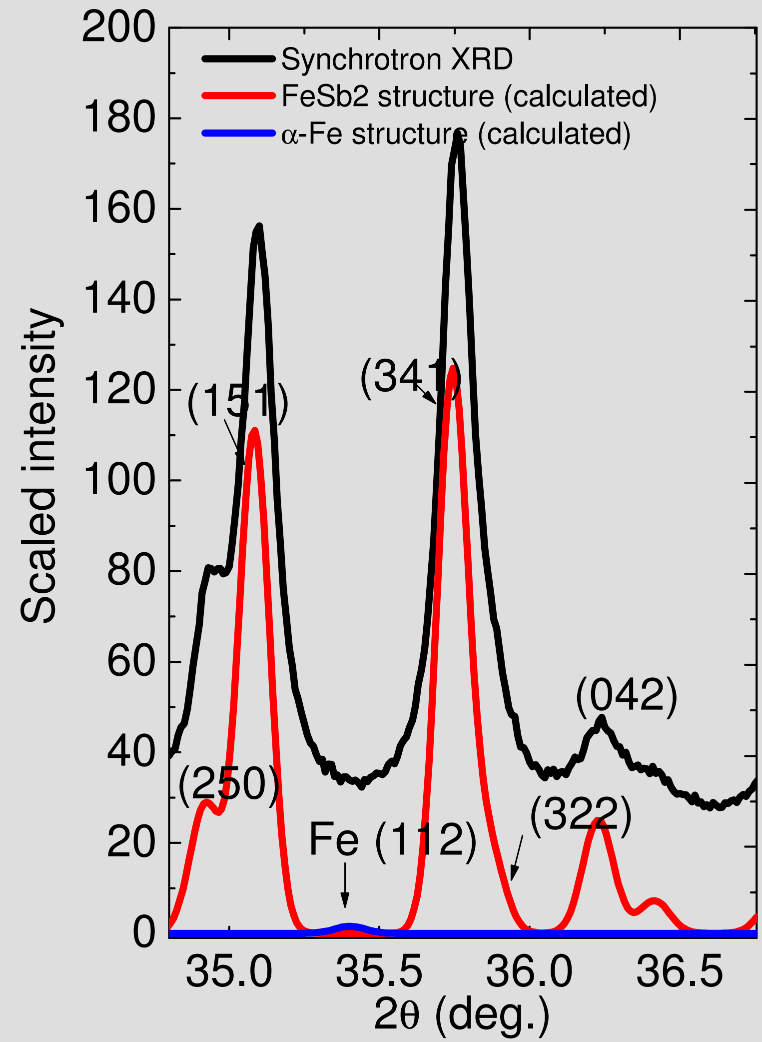
Rongwei Hu (胡荣伟) et al,
Phys. Rev. B 76, 224422 (2007)



Intrinsic WFM



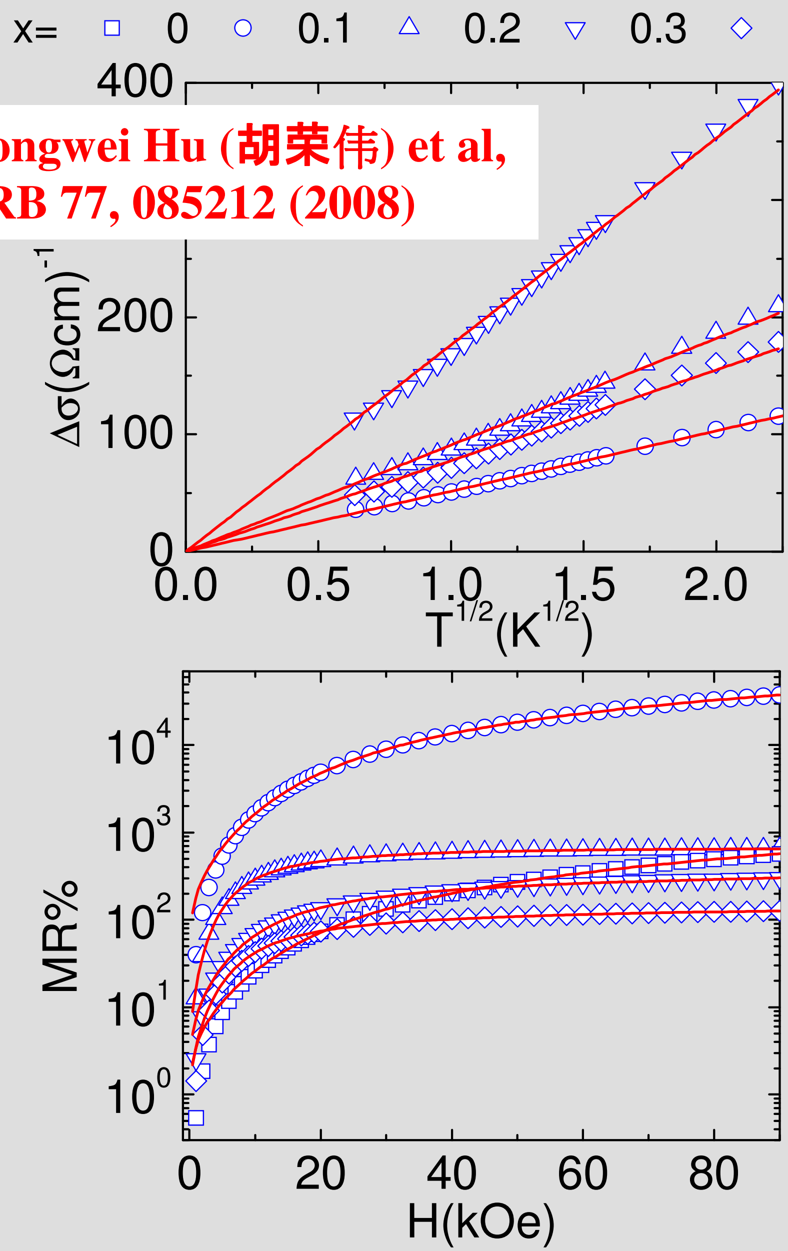




Rongwei Hu (胡荣伟) et al,
Phys. Rev. B 76, 224422 (2007)

Electronic Correlations Are Important

Rongwei Hu (胡荣伟) et al,
PRB 77, 085212 (2008)



Corrections to quadratic MR:

(P. Lee and T. V. Ramakrishnan, PRB 26, 4009 (1982);
B. Altshuler and A. G, Aronov, JETP Lett. 33, 499 (1981))

$$MR = \frac{1}{\rho_0} 0.77\alpha F \left(\frac{g\mu_B}{k_B}\right)^{1/2} H^{1/2} - \frac{\rho_0 e^2 L_f}{\pi\hbar b^2}\left[\left(1 + \frac{(bL_f)^2}{12(L_B)^4}\right)^{-\frac{1}{2}} - 1\right] + cH^2$$

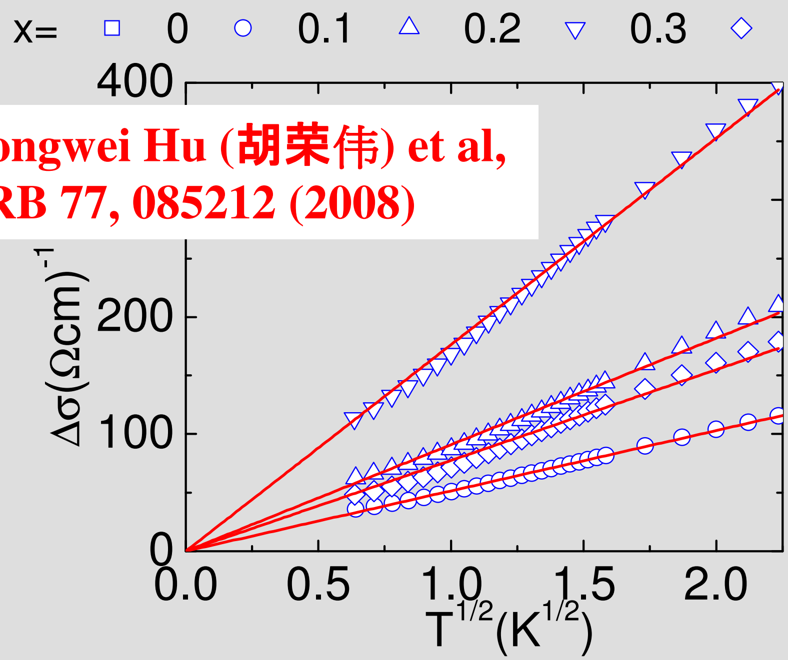
COULOMB INTERACTION

QUASI 1D WEAK LOCALIZATION

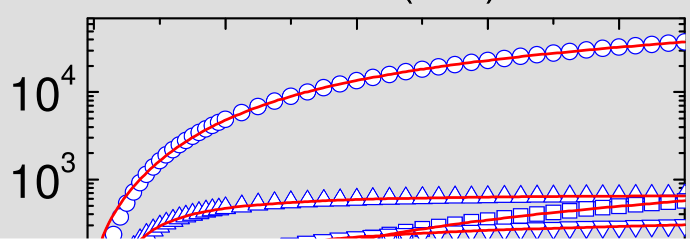
L_f: phase coherence length
$L_B=(\hbar/2eB)^{1/2}$: magnetic length
b: width of quasi 1D channel
αF: from Hartree interaction

Orbital MR in multicarrier model:
~ 10^{-4} of observed MR
Coulomb interaction + disorder:
~ 95% of observed MR

Electronic Correlations Are Important



Rongwei Hu (胡荣伟) et al, PRB 77, 085212 (2008)



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COULOMB INTERACTION

QUASI 1D WEAK LOCALIZATION

L_f: phase coherence length
$L_B=(\hbar/2eB)^{1/2}$: magnetic length
b: width of quasi 1D channel
αF: from Hartree interaction

x	αF	L_f (nm)	b (nm)	c
0	1.2×10^{-9}	162	1.6	0.001
0.1	6.2×10^{-7}	1463	0.2	0.055
0.2	5.1×10^{-9}	534	2.8	0.004
0.3	7.3×10^{-9}	188	4.0	0.002
0.4	9.9×10^{-9}	128	5.1	0.001

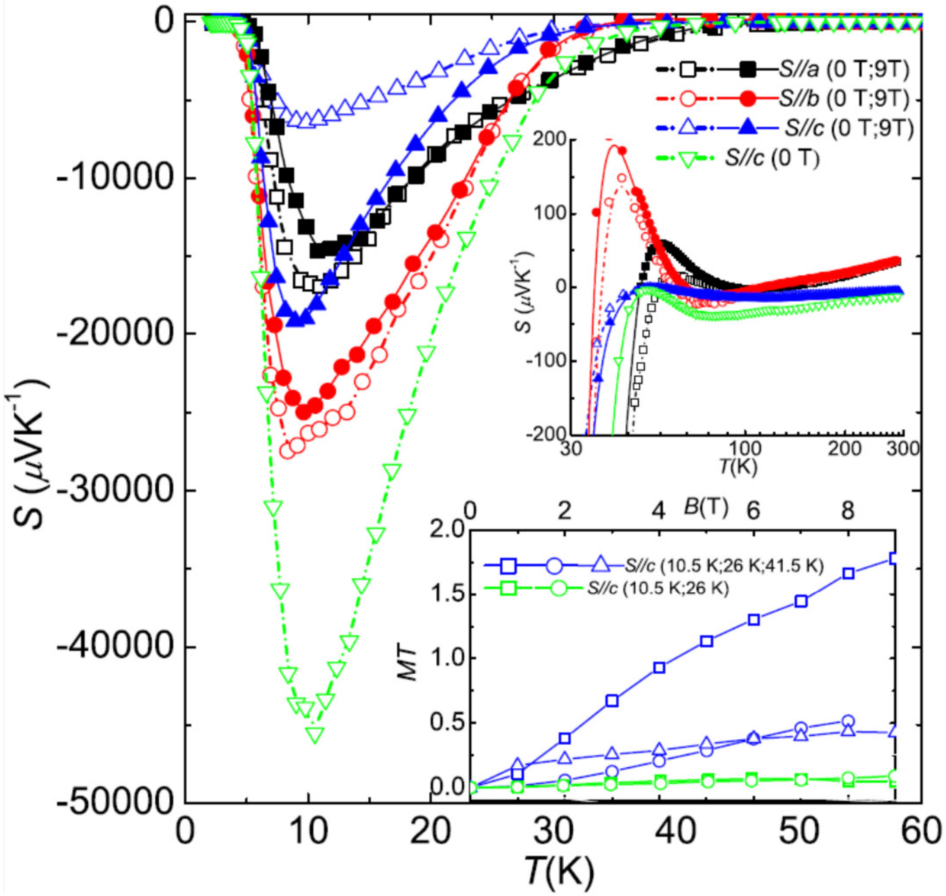
MR is positive as expected for the strong spin-orbit scattering and nearly magnetic conductors such as Pd and Pt alloys where spin subbands split so that αF is large.

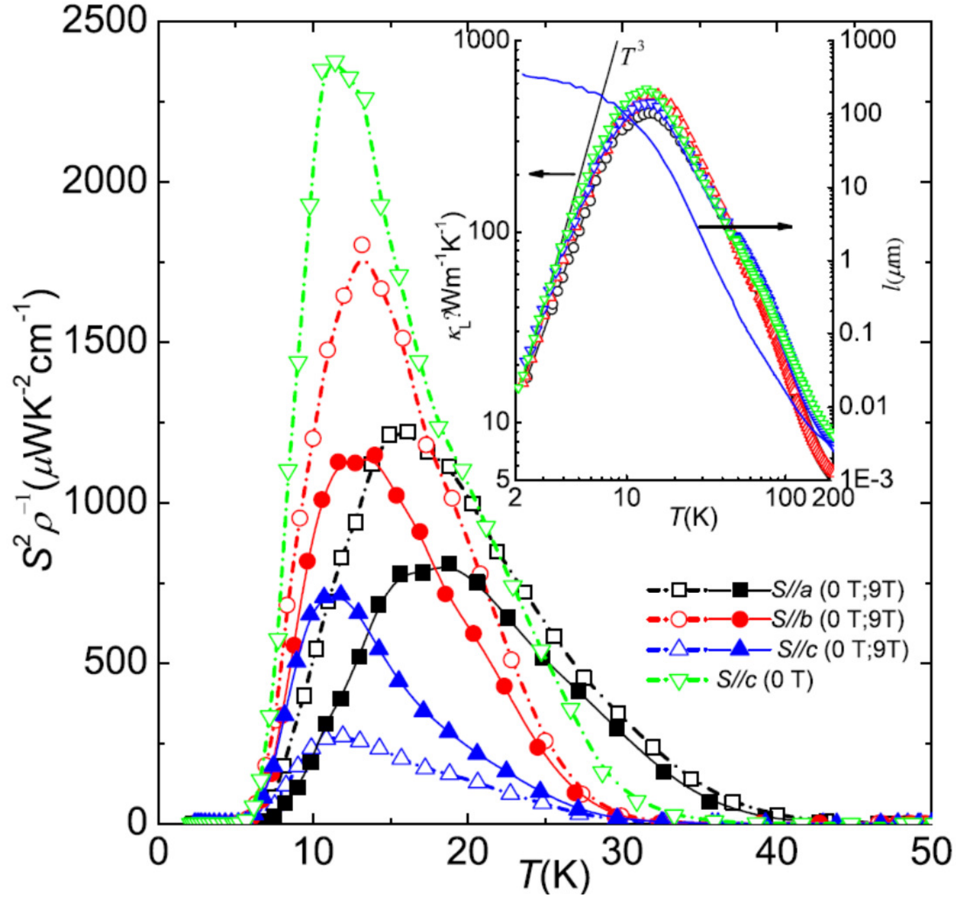
Colossal Thermopower in $FeSb_2$

A. Bentien et al., Europhys. Lett. 80, 17008 (2007)

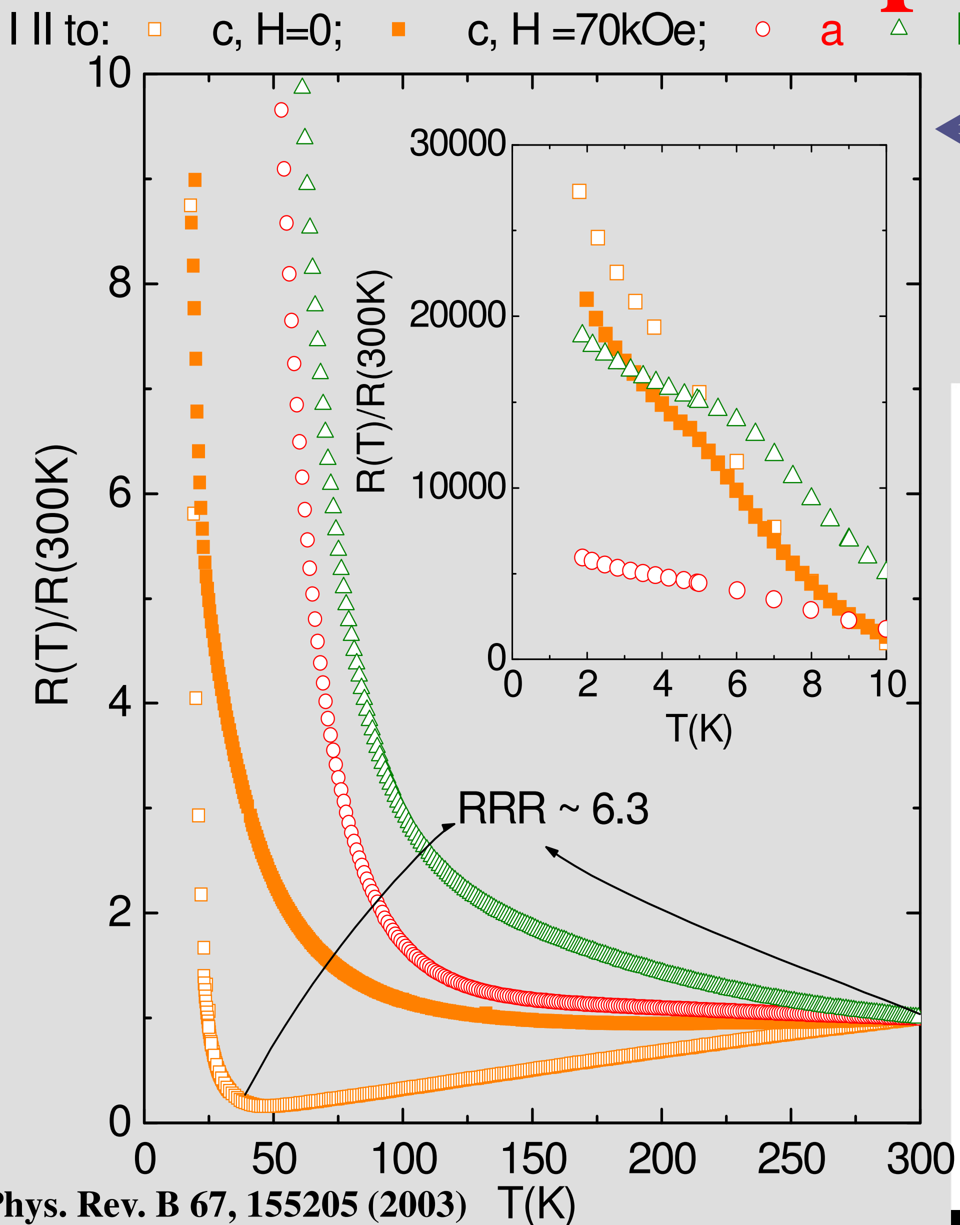
Large phonon mean free path + evidence of e-ph coupling
But phonon drag should not be dominant: S due to diffusion
(P. Sun et al., PRB B 79, 153308 (2009),
P. Sun et al.,, Dalton Trans. 39, 1012 (2010))

κ_e important above 100K
$\kappa_L = (1/3)C(T)v_s l_p \rightarrow l_p = 350\mu m$





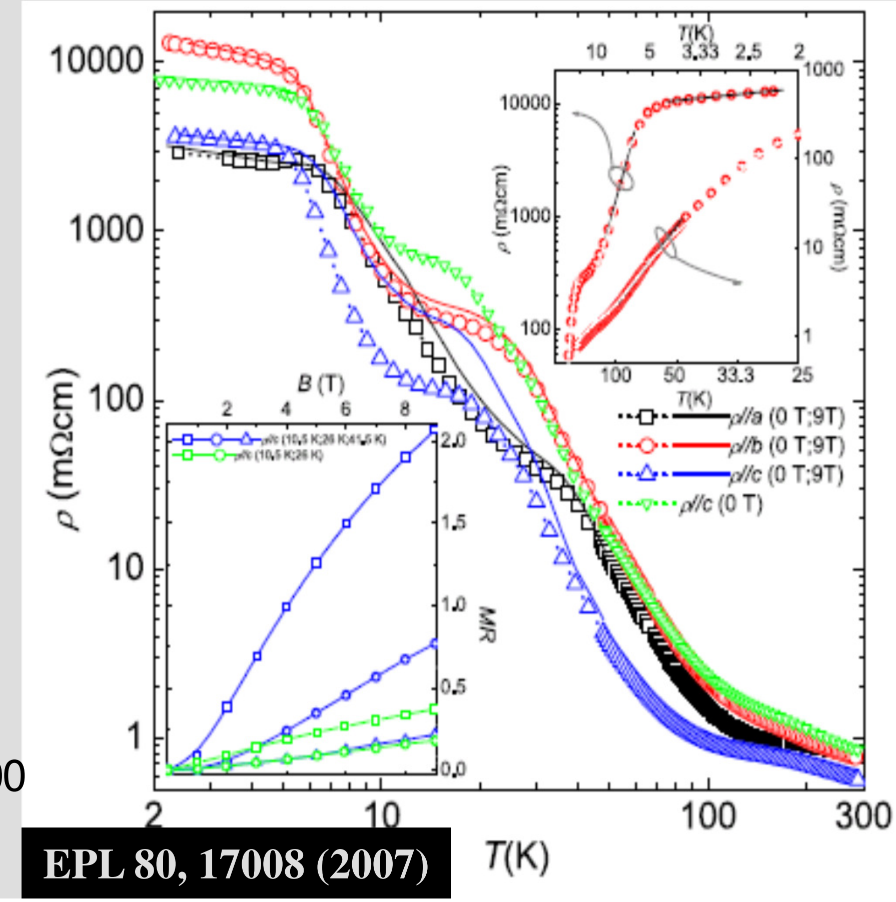
Problems: sample dependence?



Phys. Rev. B 67, 155205 (2003)
Phys. Rev. B 72, 045103 (2005)

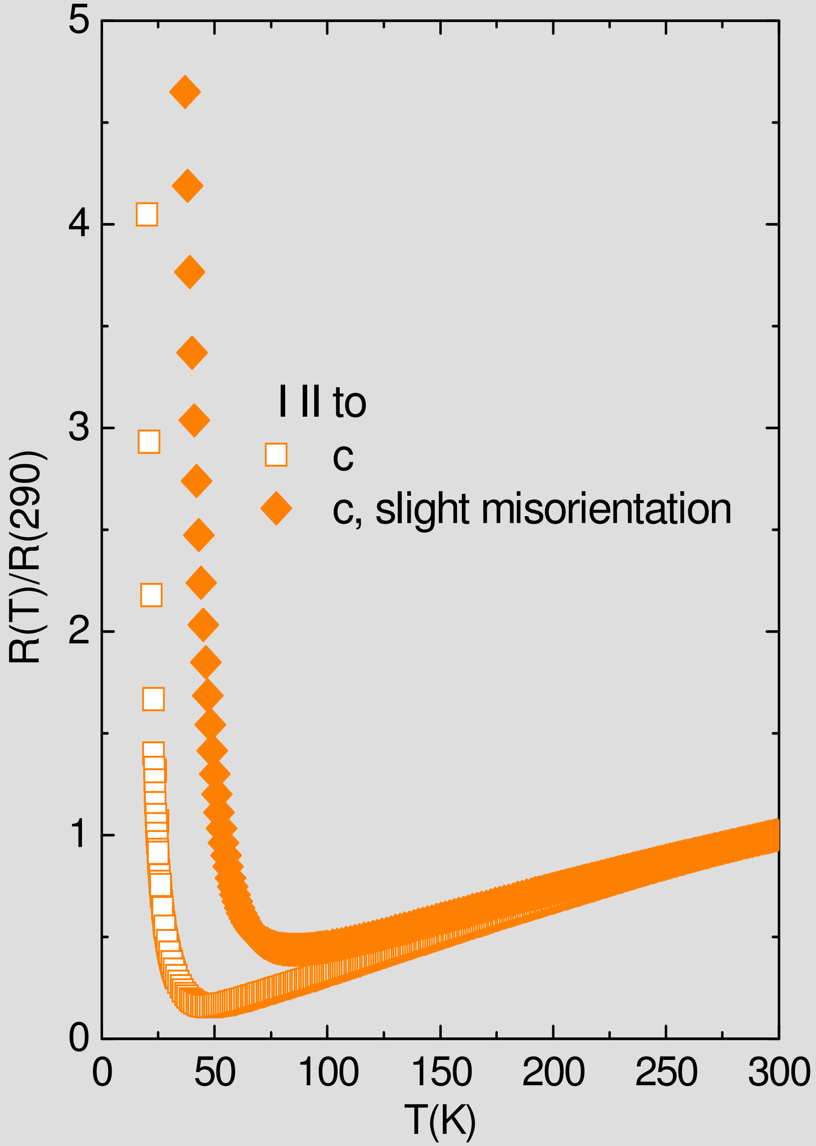
ρ(300K)=1.04mΩcm [a], 0.31mΩcm [b], 0.80mΩcm [c]

Small MR



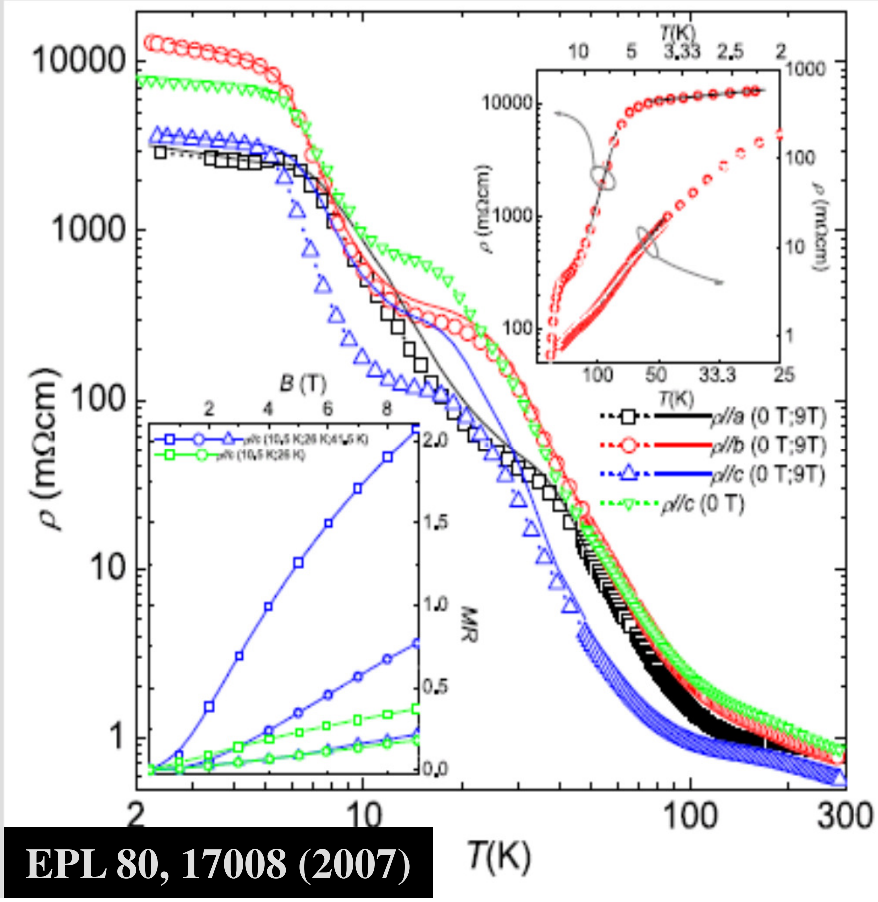
EPL 80, 17008 (2007)

Problems: sample dependence?



ρ(300K)=1.04mΩcm [a], 0.31mΩcm [b], 0.80mΩcm [c]

Small MR



Phys. Rev. B 67, 155205 (2003)
Phys. Rev. B 72, 045103 (2005)

EPL 80, 17008 (2007)

Comparison of $FeSb_2$ crystals

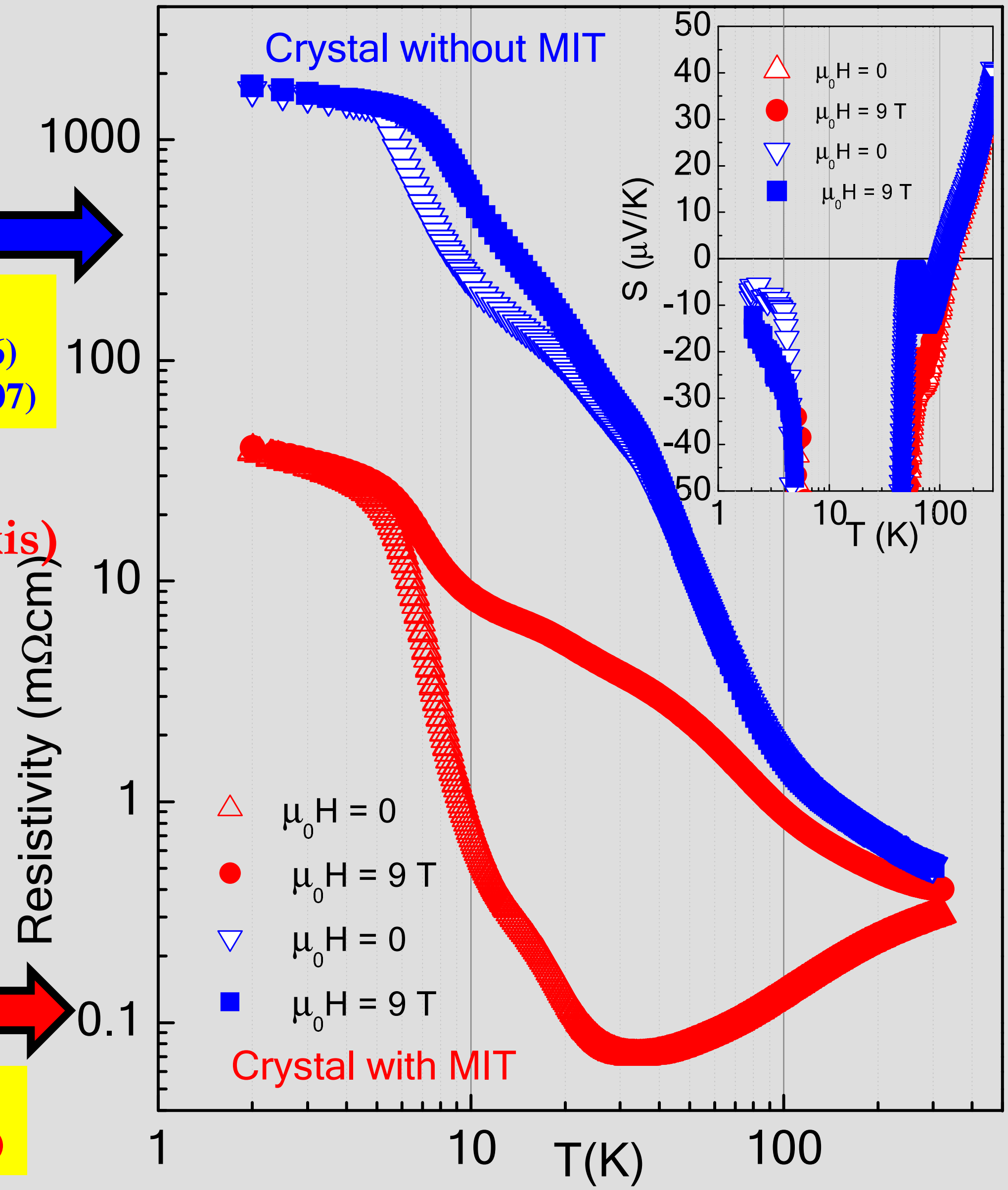
Phys. Rev. B 86, 115121 (2012)

no MIT crystal, similar to
A. Bentien et al., Phys. Rev. B 74, 205105 (2006)
A. Bentien et al., Europhys. Lett. 80, 17008 (2007)

- **Optics:**

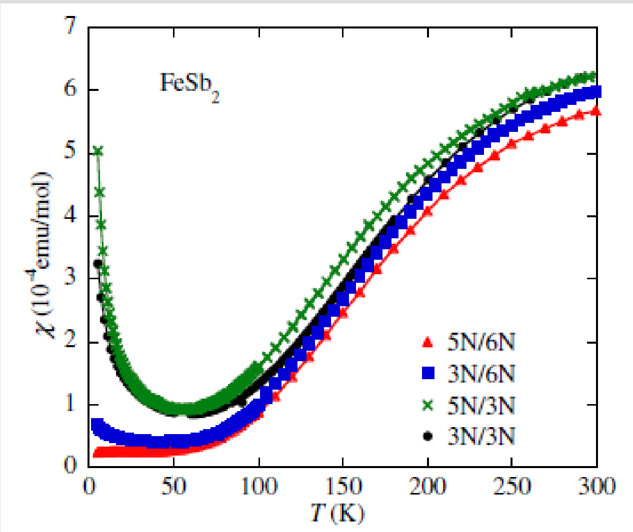
44 meV (ab), (12.5-37) meV (c –axis)
(Europhys. B 54, 175 (2006))
130meV (direct), (31 and 6) meV (indirect)
(Phys. Rev. B 82, 245205 (2010))

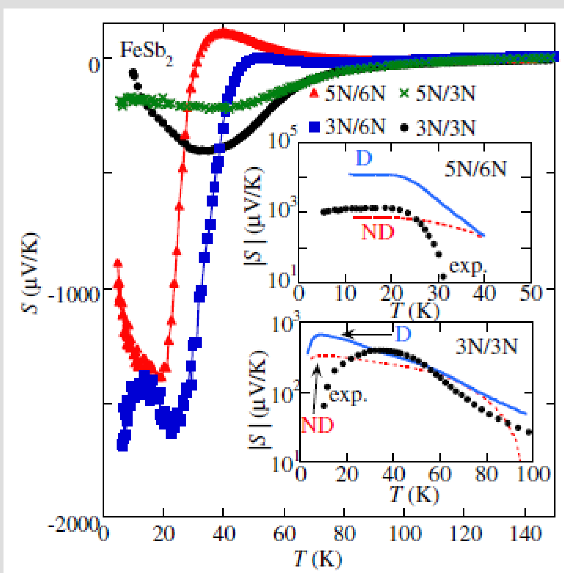
MIT crystal, similar to
C. Petrovic et al, Phys. Rev. B 67, 155205 (2003)

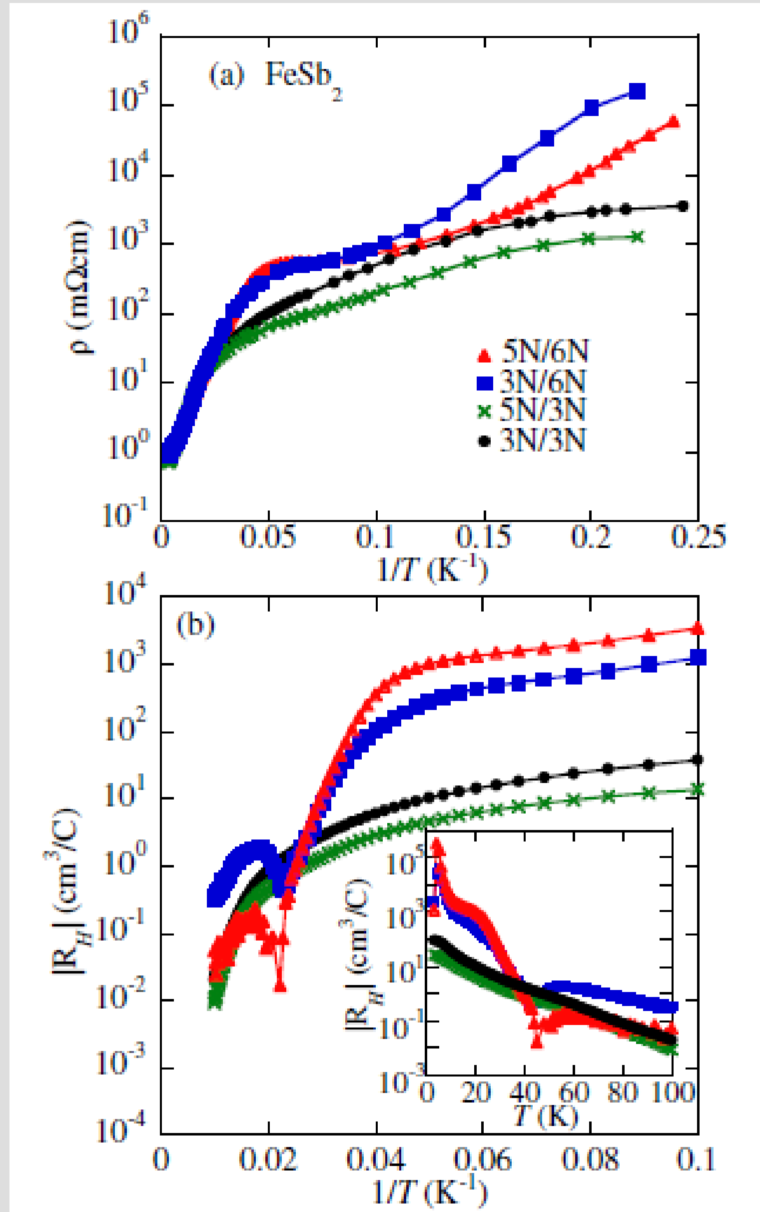


Role of Simple Impurities?

H. Takahashi et al., J. Phys. Soc. Japan 80, 054708 (2011)







$FeSb_2$ – multicarrier transport

$$R_H = -\frac{1}{H}\frac{\sum \sigma^i_{xy}}{(\sum \sigma^i_{xx})^2 + (\sum \sigma^i_{xy})^2}$$

$$\sigma^i_{xx} = \frac{q n_i \mu_i}{1+\mu_i^2 H^2}, \quad \sigma^i_{xy} = \frac{q n_i \mu_i^2 H}{1+\mu_i^2 H^2}$$

Carrier" is a set or collection of carriers having the same mobility, associated with only one energy or a degenerate energy level

two carrier system:

$$R_H = \frac{\rho_{xy}}{H} = \rho_0 \frac{\alpha_2 + \beta_2 H^2}{1+\beta_3 H^2}$$

$$\alpha_2 = f_1\mu_1 + f_2\mu_2$$

$$\beta_2 = (f_1\mu_2 + f_2\mu_1)\mu_1\mu_2$$

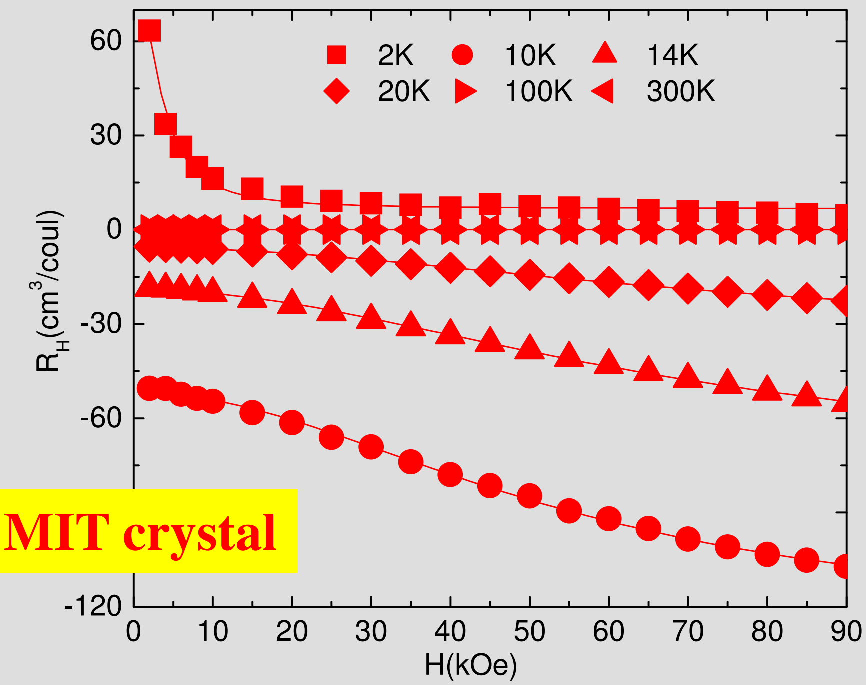
$$\beta_3 = (f_1\mu_2 + f_2\mu_1)^2$$

$$\rho_0 = \rho(B=0)$$

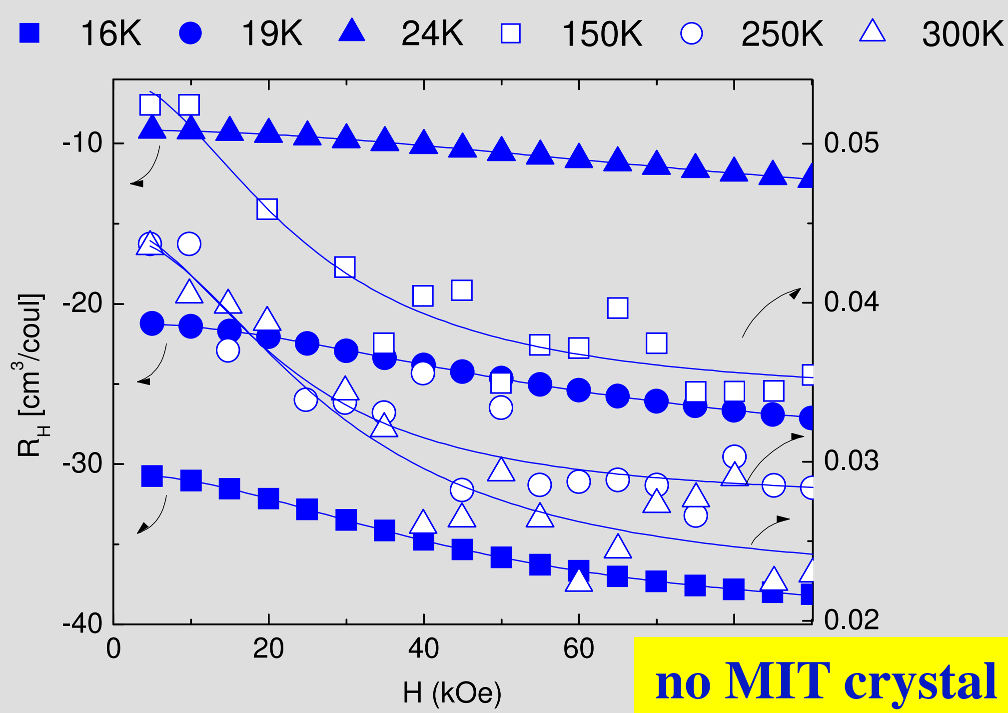
$$f_i = \frac{n_i\mu_i}{\sum |n_i\mu_i|}$$

CARRIER MOBILITIES

CARRIER CONCENTRATIONS



MIT crystal



no MIT crystal

Two band model for S

Noninteracting model

(J. Phys. Chem. Solids 29, 327 (1968)
Phys. Rev. B 77, 245204 (2008))

$$S=\frac{S_e\sigma_e+S_h\sigma_h}{\sigma_e+\sigma_h}$$

$$S_e=\frac{k_B}{e}\left[\frac{\left(\frac{5}{2}+s\right)F_{\frac{3}{2}+s}(\xi_e)}{\left(\frac{3}{2}+s\right)F_{\frac{1}{2}+s}(\xi_e)}-\xi_e\right]$$

$$S_h=\frac{k_B}{e}\left[\frac{\left(\frac{5}{2}+s\right)F_{\frac{3}{2}+s}(\xi_h)}{\left(\frac{3}{2}+s\right)F_{\frac{1}{2}+s}(\xi_h)}-\xi_h\right]$$

$$F_j(\xi)=\int_0^\infty\frac{x^j}{1+e^{(x-\xi)}}dx$$

Relaxation time energy dependence: $\tau=\tau_0E^S$
$\xi=E_F/k_BT$; $E_F=(h^2/2m^*)(N/V)^{2/3}(3/8\pi)^{2/3}$
and
$E_{Fe} = -E_{Fh}+E_g$; $\xi_e = -\xi_h-E_0/k_BT$; $m^*=m_e$
and
s = -1/2 (acoustic phonon scattering is dominant)

Interacting model

Phys. Rev. B 82, 185104 (2010)

$$S=\frac{1}{|e|T}\left(\varepsilon_F-\frac{\Delta}{2}\delta\lambda\right)-\frac{5k_B}{2|e|}\delta\lambda$$

assymetry parameter →

$$\delta\lambda=\frac{\lambda^c-\lambda^v}{\lambda^c+\lambda^v};\lambda_{c,v}=\frac{Z_{c,v}^2 m_{c,v}^{*(5/2)}e^{\pm\beta\mu}}{\Gamma_{c,v}m_0^2}$$

quasiparticle weights

scattering amplitudes

In this model different band narrowings (m*) enter not only via δλ but also via ε_F:

$$\varepsilon_F=\left(\frac{3k_BT}{4}\right)\ln\left(\frac{m_v^*}{m_c^*}\right)$$

$$m_{c,v}^*=\frac{e\tau_{c,v}}{\mu_{c,v}}$$

→

$$\frac{Z_{c,v}^2\tau_{c,v}^{5/2}}{\Gamma_{c,v}}$$

becomes fit parameter, in addition to ε_F

Two band model for S

Noninteracting model

(J. Phys. Chem. Solids 29, 327 (1968)
Phys. Rev. B 77, 245204 (2008))

$$S = \frac{S_e\sigma_e + S_h\sigma_h}{\sigma_e + \sigma_h}$$

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$$S_h = \frac{k_B}{e}\left[\frac{\left(\frac{5}{2}+s\right)F_{\frac{3}{2}+s}(\xi_h)}{\left(\frac{3}{2}+s\right)F_{\frac{1}{2}+s}(\xi_h)} - \xi_h\right]$$

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$\xi=E_F/k_BT$; $E_F=(h^2/2m^*)(N/V)^{2/3}(3/8\pi)^{2/3}$
and
$E_{Fe} = -E_{Fh}+E_g$; $\xi_e = -\xi_h - E_0/k_BT$; m*=m
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s = -1/2 (acoustic phonon scattering is dom

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Phys. Rev. B 82, 185104 (2010)

$$S = \frac{1}{|e|T}\left(\varepsilon_F - \frac{\Delta}{2}\delta\lambda\right) - \frac{5k_B}{2|e|}\delta\lambda$$

assymetry parameter

$$\delta\lambda = \frac{\lambda^c - \lambda^v}{\lambda^c + \lambda^v};\ \lambda_{c,v} = \frac{Z_{c,v}^2 m_{c,v}^{*(5/2)} e^{\pm\beta\mu}}{\Gamma_{c,v} m_0^2}$$

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scattering amplitudes

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$$\varepsilon_F = \left(\frac{3k_BT}{4}\right)\ln\left(\frac{m_v^*}{m_c^*}\right)$$

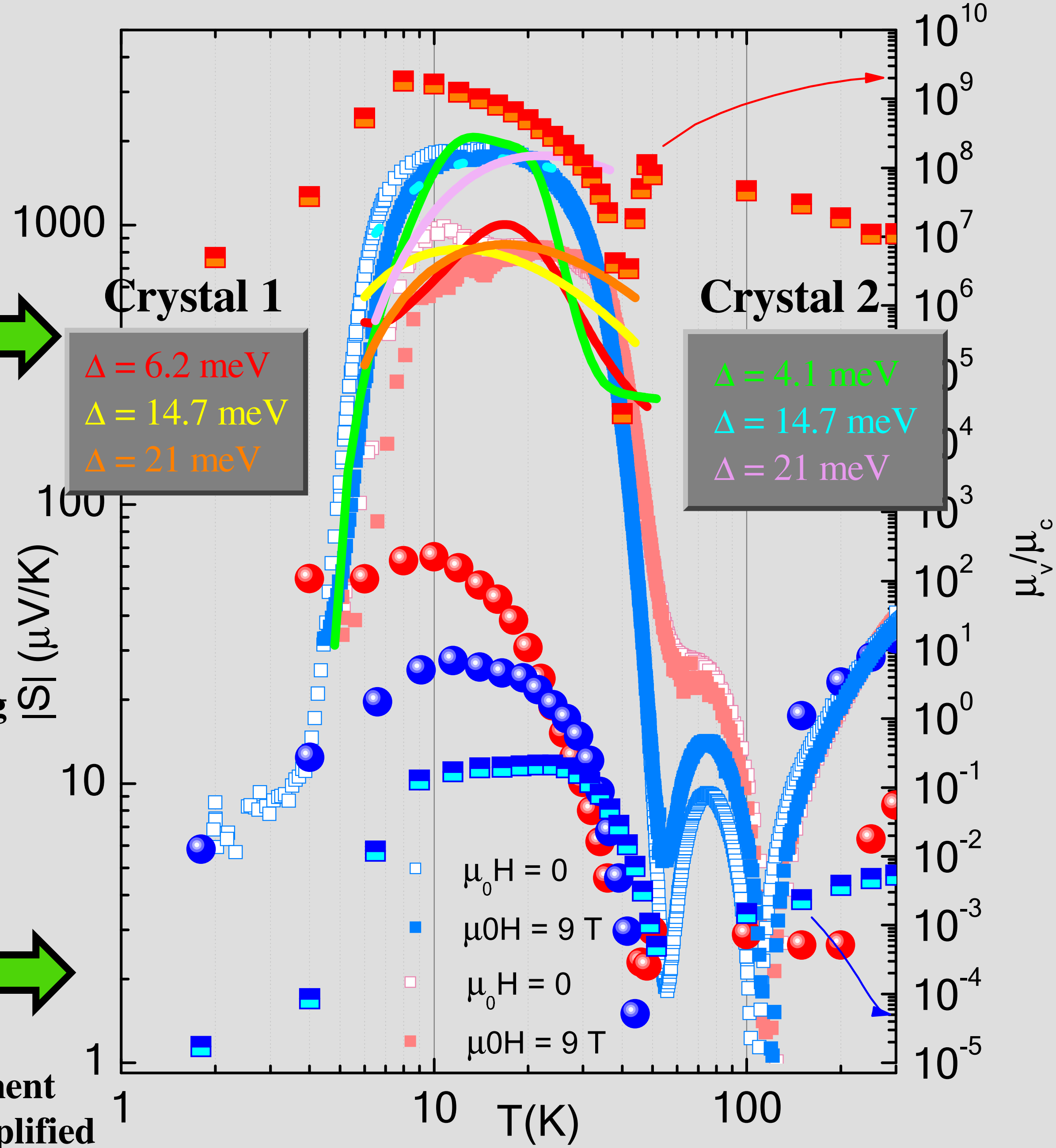
$e\tau$

$Z^2\ \tau^{5/2}$

becomes fit

(2-5)K	(10 - 30)K	(80 - 100)K	ZΓ	ϵ_F
0.14(1) meV	6.2(1) meV	metallic	$6.2\cdot10^{-8}$	3.4 meV
0.08(1) meV	4.1(1) meV	14.7(1) meV	38	0.8 meV

Two band model for S: fits



Note gap values: large S best fit with a gap of about ~ 20 meV

Correlated electron effects vane at high temperarues: noninteracting model is a good aproximation

Similar to magnetoresistance, S in the region of large enhancement has similar T dependence but is amplified

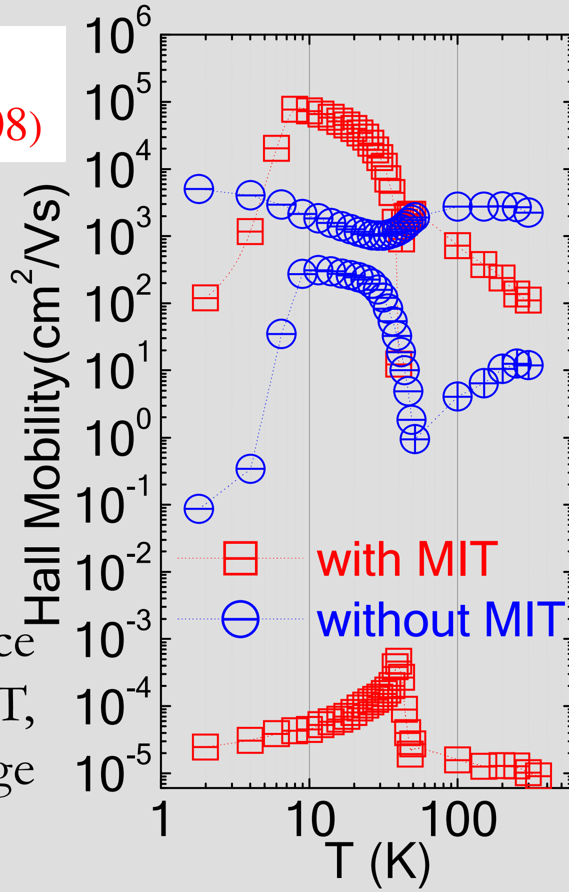
Back to Two Band Conduction

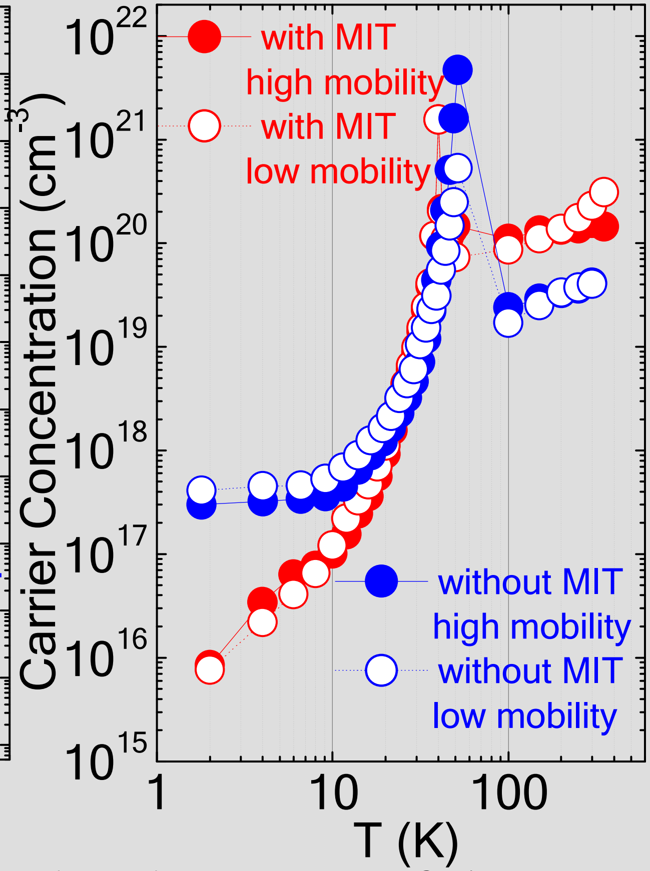
Rongwei Hu (胡荣伟) et al,
Appl. Phys. Lett. 92, 182108 (2008)

Crystal with MIT: $\mu_v >> \mu_c$

Crystal with no MIT: opposite $\mu_c >> \mu_v$

But, temperature dependence similar and with anomaly at MIT, both bands with holes change sign below MIT

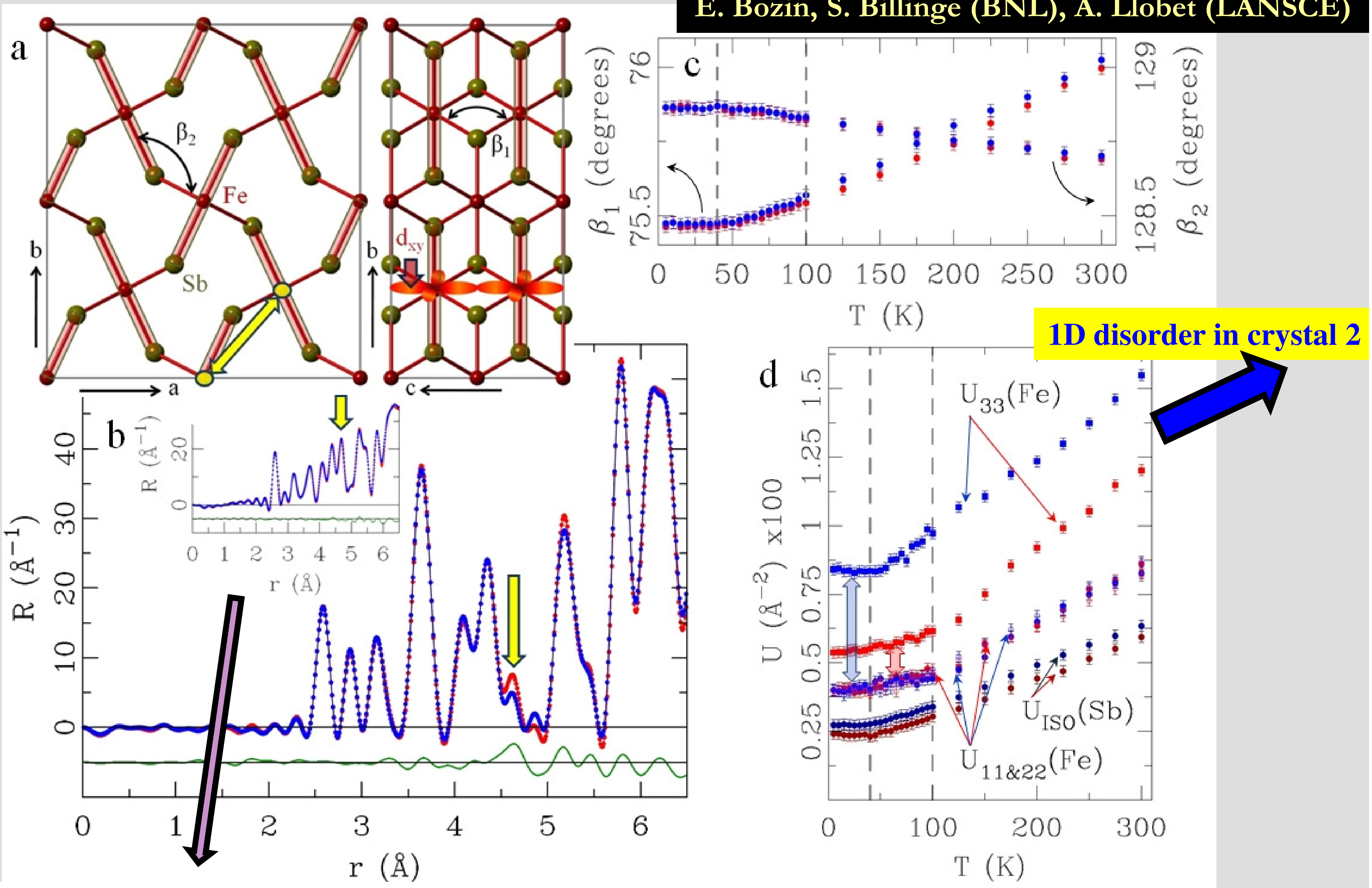




Lowest unoccupied states are from d_{xy}: nonbonding and overlap along c axis of the crystal (chains of edge sharing octahedra) forming quasi 1D band → **<u>MIT sample ρ above 40 K due to holes in nearly filled valence band.</u>** **At MIT d_{xy} is depleted and attains half filling in crystal 1, whereas disorder in crystal 2 inhibits metallicity due to localization, impacts the d_{xy} overlap and orbital dependent Hubbard U in d_{xy} band of itinerant states**

X ray PDF: Local Structure Differences

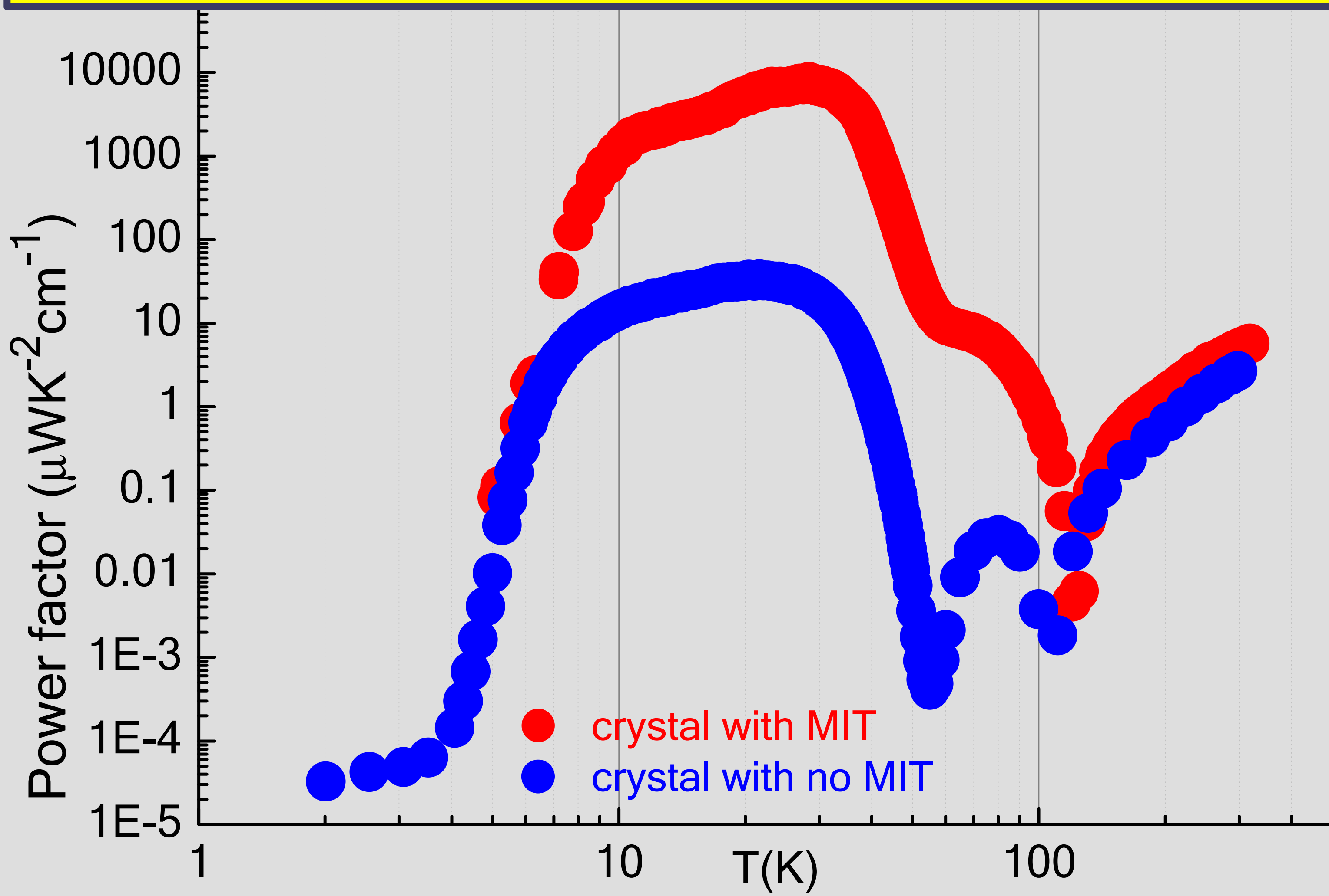
E. Bozin, S. Billinge (BNL), A. Llobet (LANSCE)



Neutron PDF: Identical local structure

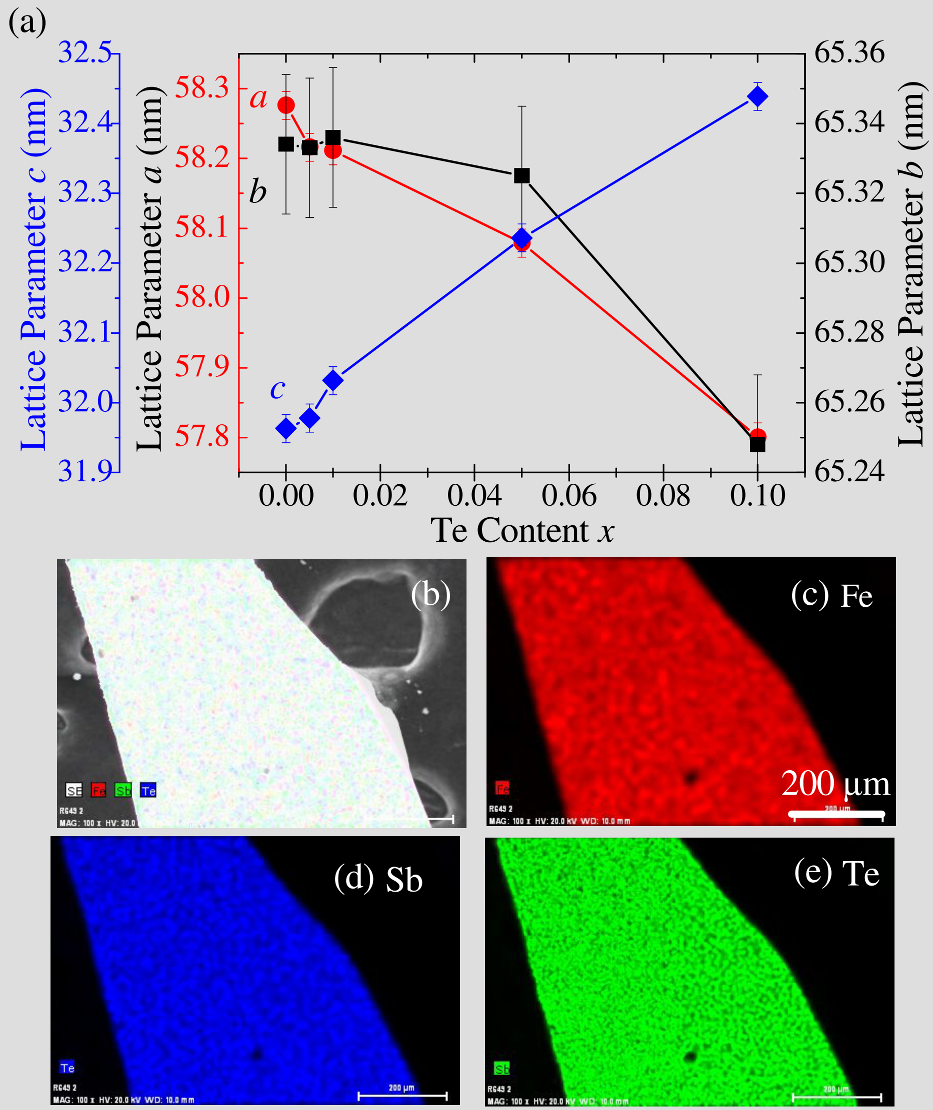
Increase in Thermoelectric Power Factor

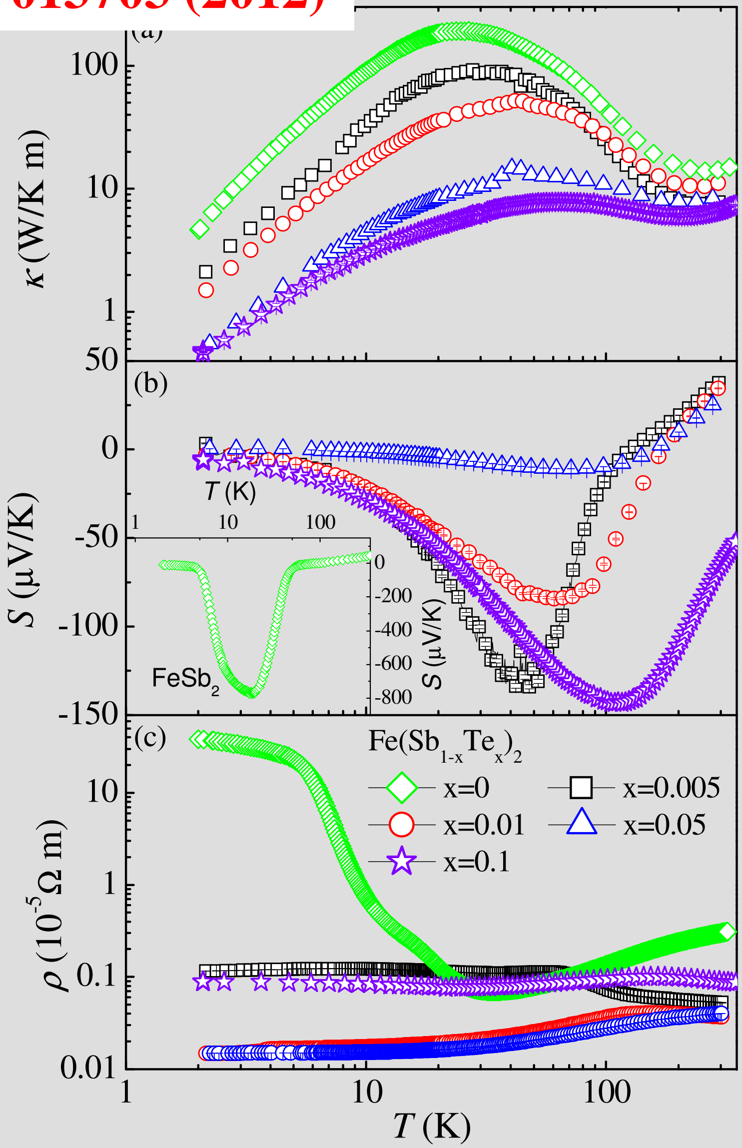
Qing Jie, Rongwei Hu (胡荣伟) et al, Phys. Rev. B 86, 115121 (2012):
Highest known thermoelectric power factor
(ELECTRONIC CORRELATIONS AND DISORDER)



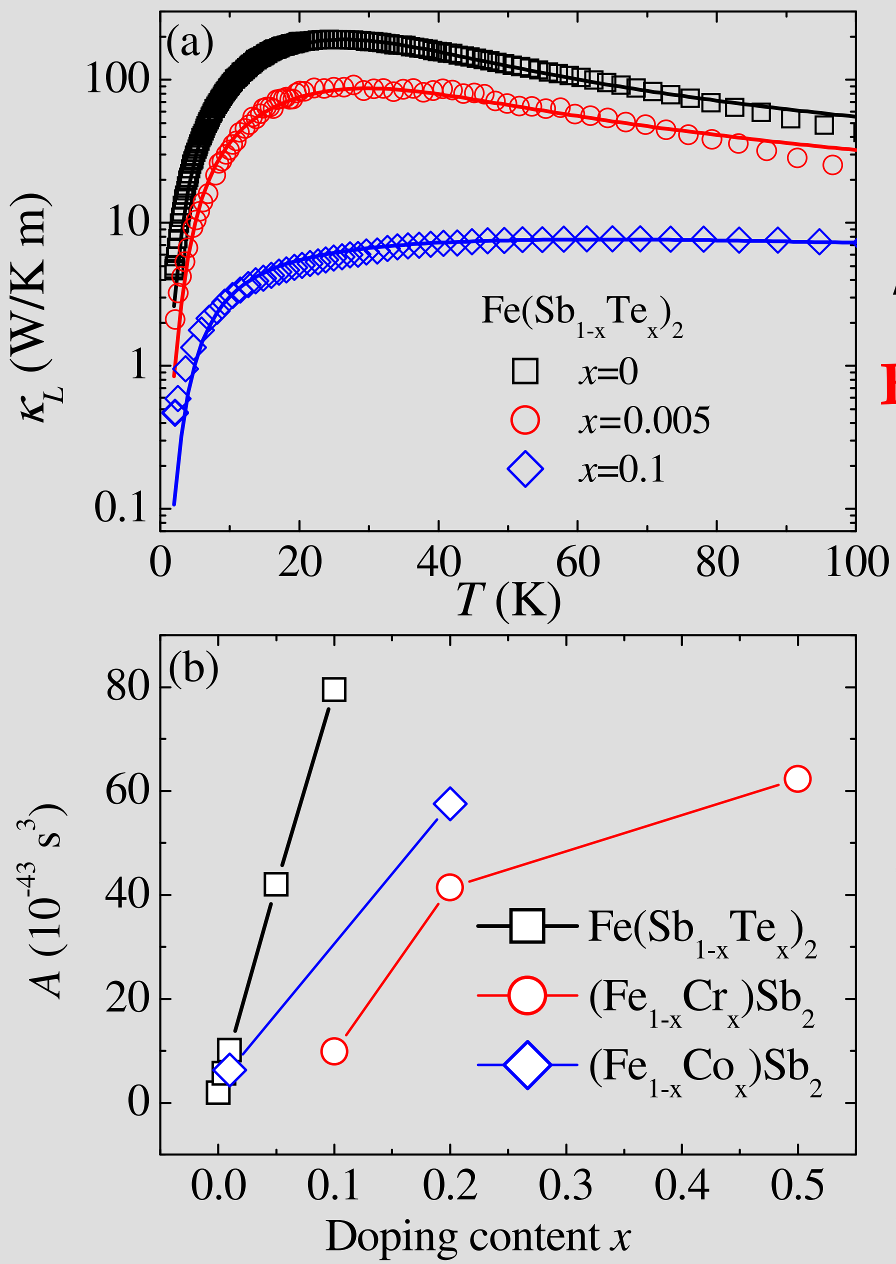
$Fe(Sb_{1-x}Te)_2$: Reduction of κ

Kefeng Wang (王克锋) et al, J. Appl. Phys. 112, 013703 (2012)





$Fe(Sb_{1-x}Te_x)_2$



$$\kappa_L = \frac{k_B}{2\pi^2 v}\left(\frac{k_B}{\hbar}\right)^3 \int_0^{\theta_D/T} \frac{\tau_C x^4 e^x}{e^x - 1} dx$$

Boundary **Defect**

$$\tau_C^{-1} = \tau_B^{-1} + \tau_D^{-1} + \tau_U^{-1}$$

Umklapp

$$\tau_C^{-1} = \frac{v}{L} + A\omega^4 + B\omega^2 T e^{-\theta_D/3D}$$

$$\mathbf{A = \Omega_0\Gamma/4\pi v^3 \qquad \Gamma=\Gamma_M+\Gamma_S}$$

Nominal x	Actual x	L (μm)	A (10^{-43} s^3)	B (10^{-18} s K^{-1})
		$Fe(Sb_{1-x}Te_x)_2$		
0	…	72	1.9	2.4
0.005	0.006(7)	23	5.6	3.8
0.01	0.007(9)	51	10.1	2.1
0.05	0.04(3)	42	40.7	3.5
0.1	0.09(1)	67	79.5	2.7

Kefeng Wang (王克锋) et al, J. Appl. Phys. 112, 013703 (2012)

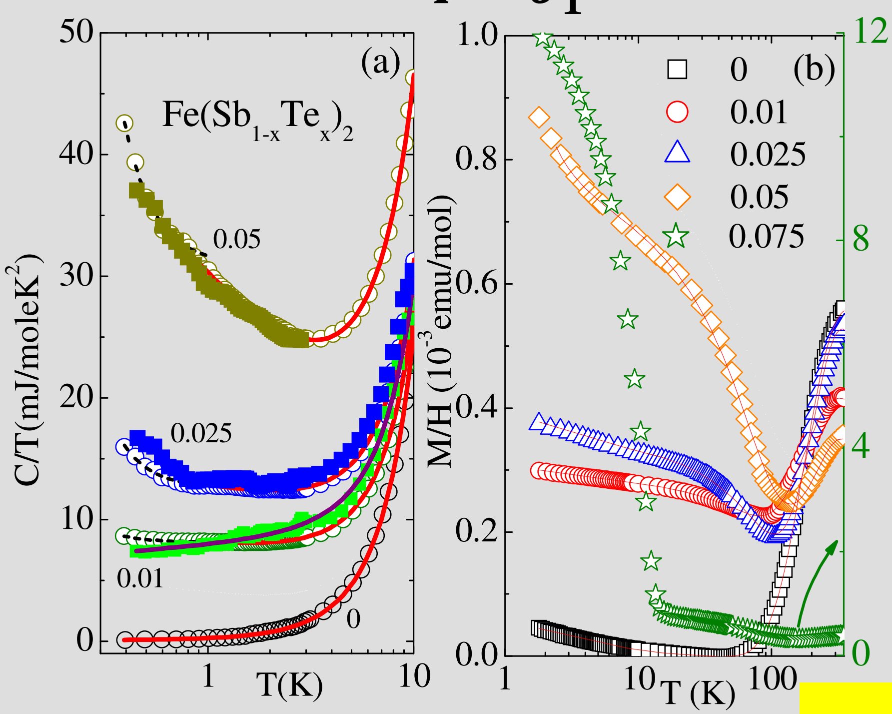
Electronic Griffiths Phase in $Fe(Sb_{1-x}Te)_2$

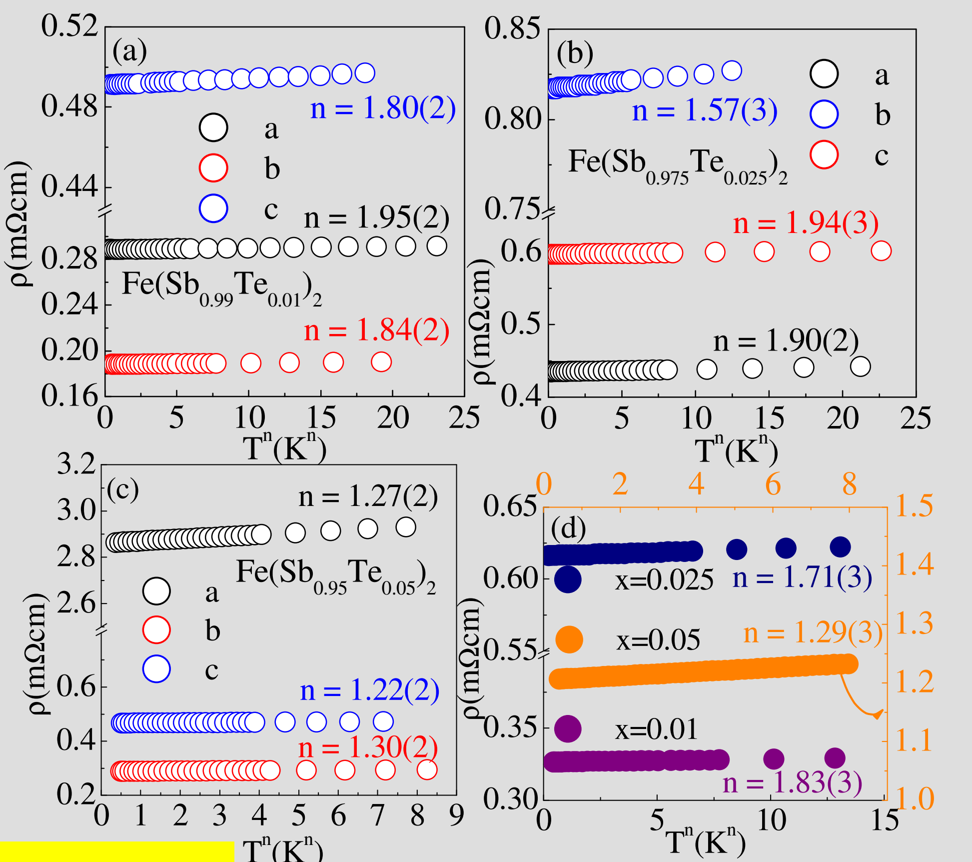
x	$\Delta(K)$	$W(K)$	$\mu_1(\mu_B)$	Θ_1 (K)	a	λ_χ	λ_C	γ_0 (mJ/molK^2)	β	δ	c	$N(E_F)$	$m^*(m_e)$	R_W
0	425(9)	310(8)	0.030(2)	0.8(2)				~ 0	0.16(1)	0.0008(9)		0.0039(4)		
0.01	436(7)	451(6)	0.035(3)	1.6(3)	856(9)	0.86(3)	0.91(7)	8.7(2)	0.12(7)	0.0007(6)	8.1(8)	3.7(2)	21(1)	2.7
0.025	448(4)	525(9)	0.036(1)	3.7(3)	1117(3)	0.84(2)	0.87(5)	13.9(3)	0.15(9)	0.0005(9)	12.8(9)	5.9(3)	25(1)	2.1
0.05	453(5)	525(9)	0.039(2)	1.8(5)	1078(9)	0.89(4)	0.72(3)	39.2(3)	0.27(3)	0.0002(1)	30.2(8)	16.7(4)	56(2)	2.3

$$\frac{C(T)}{T} = \beta T^2 + \delta T^4 + cT^{-1+\lambda_C}$$

Rongwei Hu (胡荣伟) et al., PRL in press (2012)

$$\chi(T) = \chi_{NB}(T) + \frac{C_1}{T-\theta_1} + aT^{-1+\lambda_\chi}$$





unpublished

Electronic Griffiths Phase in $Fe(Sb_{1-x}Te)_2$

$$S = \frac{(\pi k_B)^2}{2e}\frac{T}{T_F} = \frac{\gamma T}{ne}$$

$$\gamma = \frac{C_{el}}{T}\frac{\pi^2 n k_B}{T_F}$$

Scaling: $q = \frac{S N_{av} e}{T\gamma} = \pm 1$

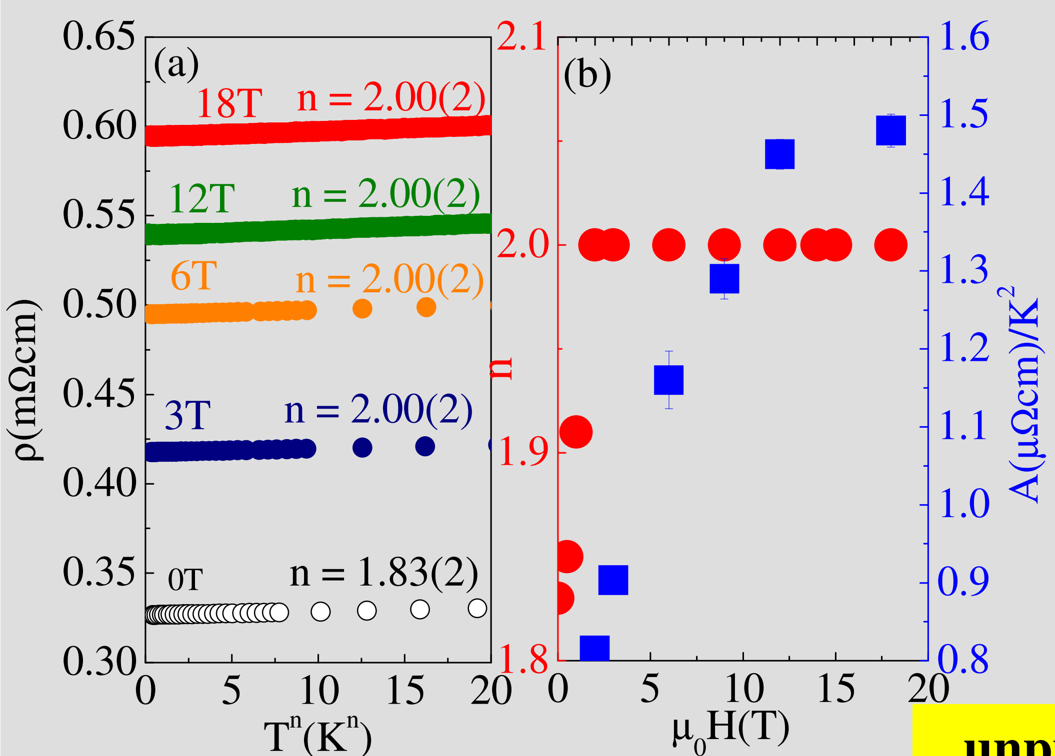
In metals with $n \sim N_{Av}$ and parabolic bands as $T \rightarrow 0$:

$S/T \sim n^{-\mu}$ and $\gamma \sim n^{\varepsilon}$ ($\mu=2/3$, $\varepsilon=1/3$, $\mu+\varepsilon=1$)

Near MIT from metallic side modified, eg. $FeSi_{1-x}Al_x$:

$(S/T) \sim \gamma^{-0.9}$ (PRB 78, 075123 (2008))

Rongwei Hu (胡荣伟) et al., PRL in press (2012)



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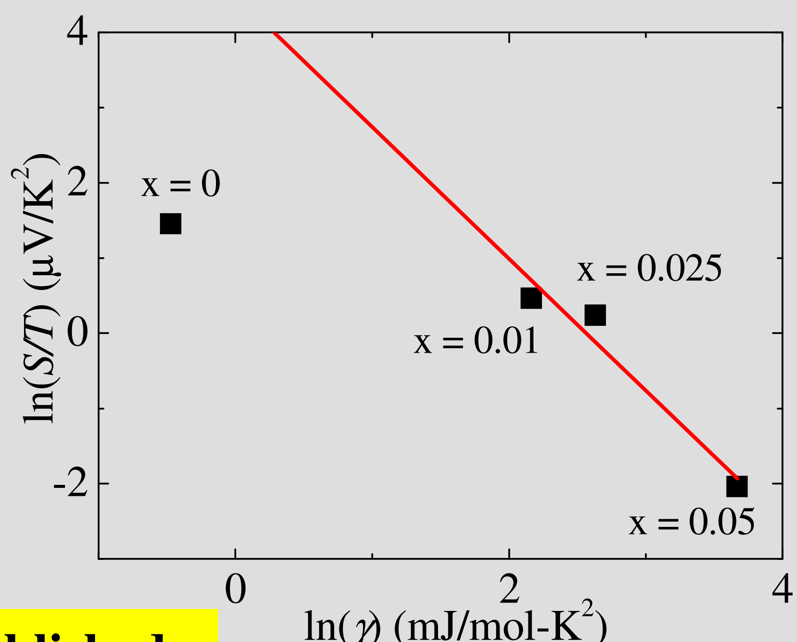

Conclusions

- **New model material created.**
- **Heavy Fermion state, intrinsic WFM and Metal-Insulator transition with doping.**
- **CMR in $Fe_{1-x}Co_xSb_2$: correlated electron disorder and localization in quasi-1D conducting channel.**
- **Electronic Seebeck and largest known thermoelectric power factor. MIT more important than S.**
- **Electronic Griffiths phase near MIT in $Fe(Sb_{1-x}Te_x)_2$**