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Title: Optical spectroscopy of Fe-based superconductors and Weyl semimetals

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Optical spectroscopy of Fe-based superconductors and Weyl semimetals

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MPA-CINT
Los Alamos National Laboratory

06/01/2016
NHMFL, Tallahassee

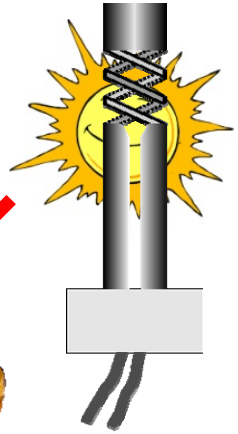
Outline

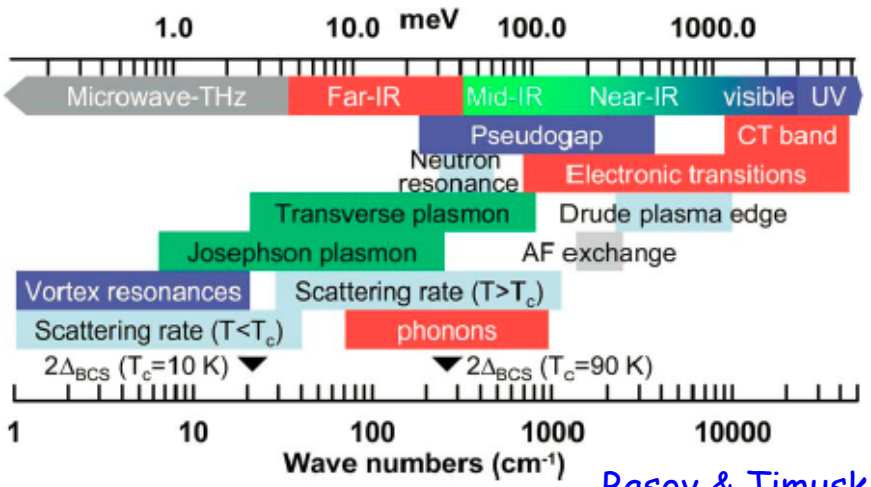
- ✓ Optical spectroscopy
- ✓ Fe-based superconductors
- ✓ 1. Hidden NFL in $Ba_{1-x}K_xFe_2As_2$
- ✓ 2. FL-NFL-FL crossover in $LiFe_{1-x}Co_xAs$
- ✓ Weyl semimetals
- ✓ 1. Signatures of Weyl points in TaAs
- ✓ 2. Ultrafast dynamics in WTe_2
- ✓ Summary

Optical spectroscopy

Detector

Light source

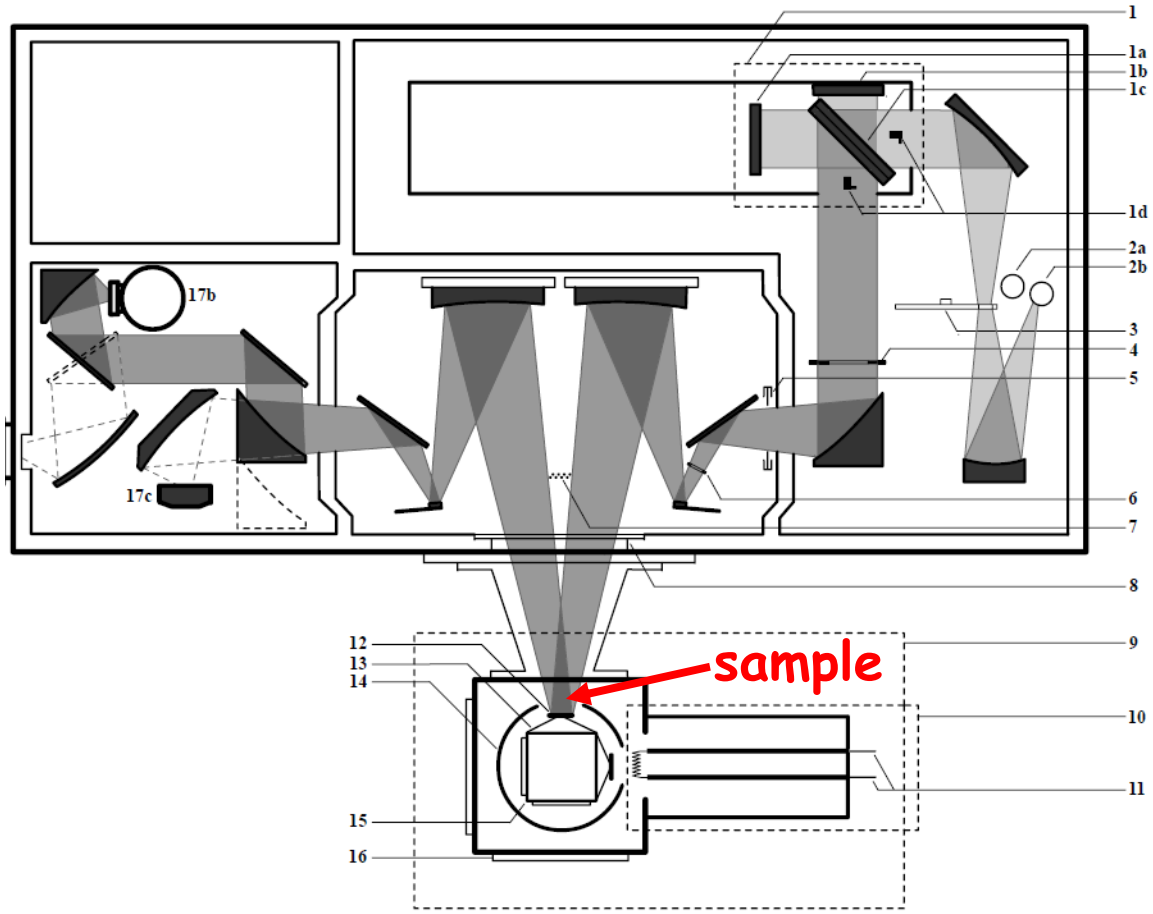




Sample

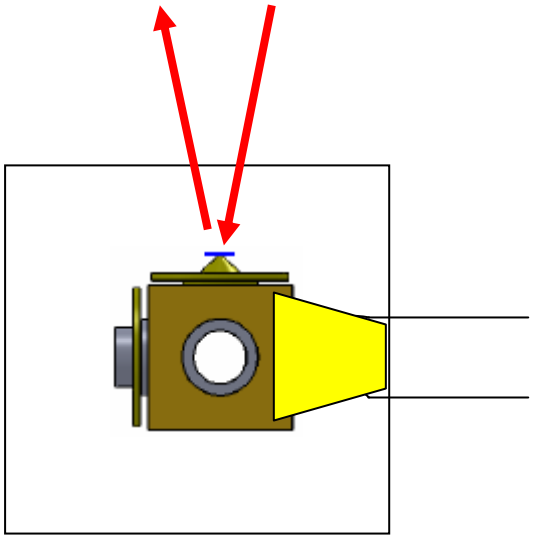
Basov & Timusk RMP **77**, 721 (2005)

Reflectivity measurements



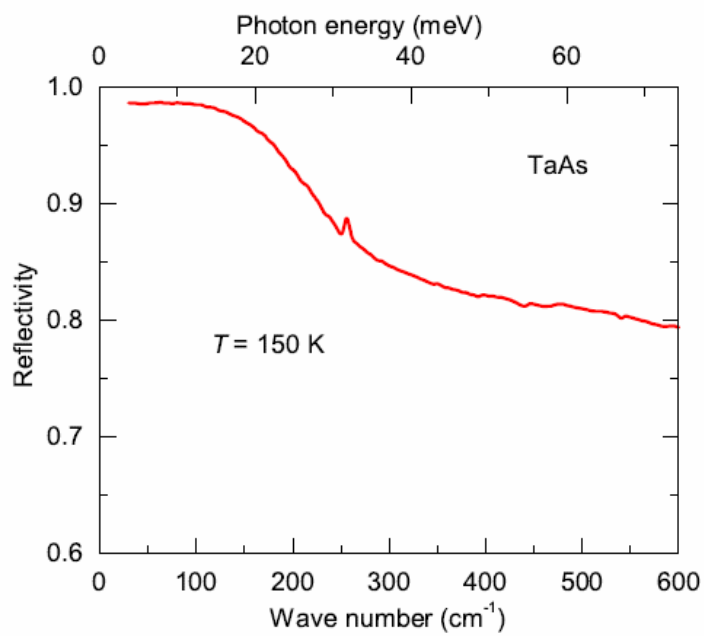
FTIR
Bruker IFS 66v

$$R(\omega) = \frac{I_{Sam}}{I_{Au}} \times R_{Au}$$



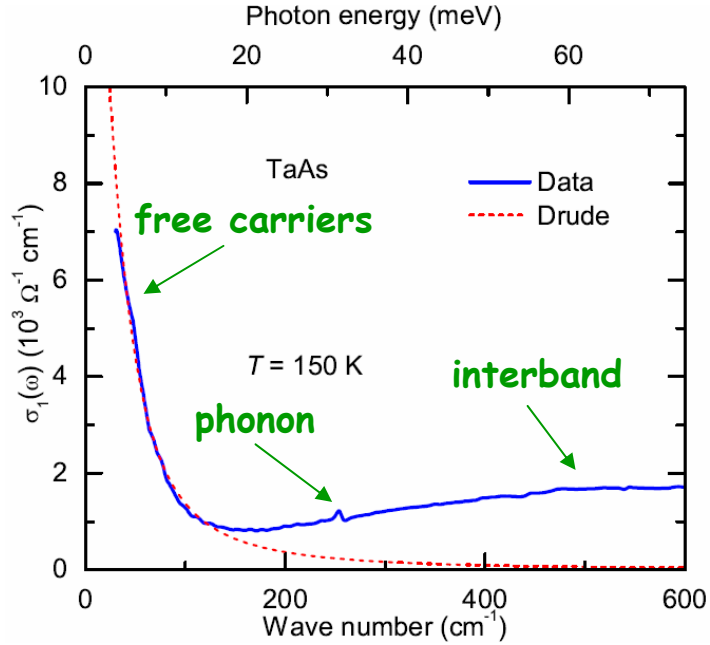
In situ gold evaporation technique

Optical conductivity



Xu and Dai *et al.* PRB **93**, 121110(R) (2016)

Kramers-Kronig



Kramers-Kronig

Reflectivity ⇨ **Phase**

↘ ↙

complex optical constants

Optical conductivity

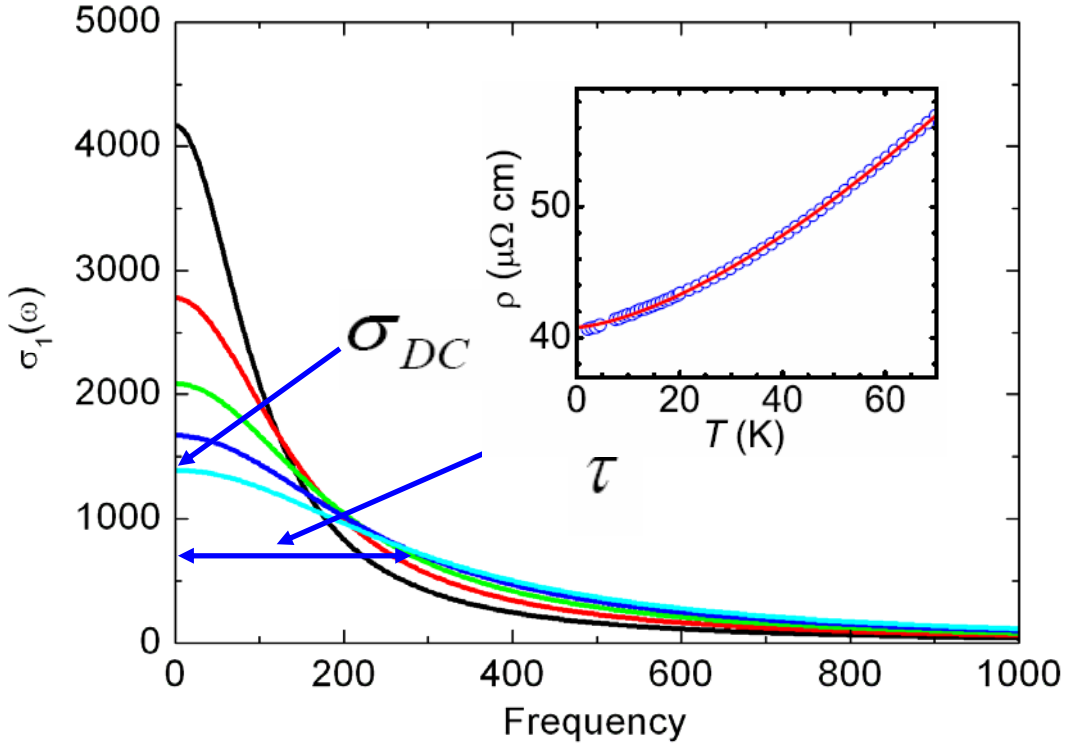
Linear superposition of independent excitations:

- ✓ **free carriers (Drude)**
- ✓ **Phonons**
- ✓ **interband transitions**

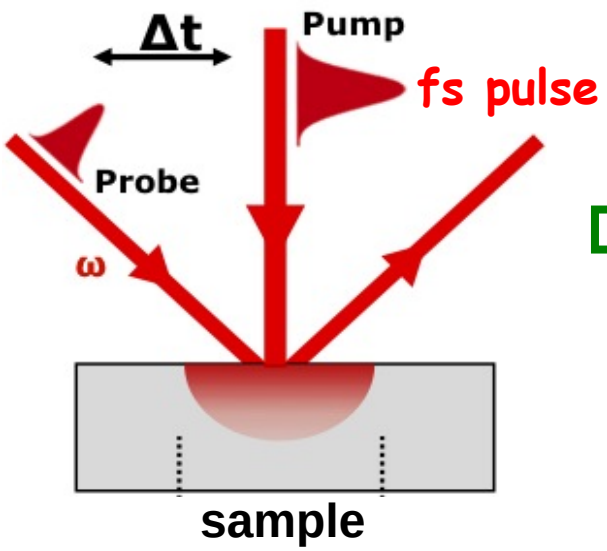
Drude model

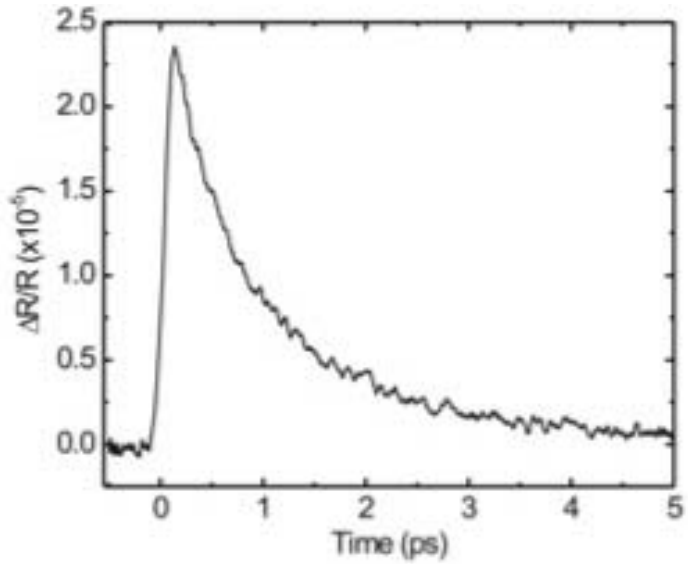
$$\sigma(\omega) = \frac{2\pi}{Z_0}\frac{\Omega_p^2}{\tau^{-1} - i\omega} = \frac{\sigma_0}{1 - i\omega\tau}$$

Optical response of
Free carriers (metals)



Pump-probe ultrafast optical spectroscopy





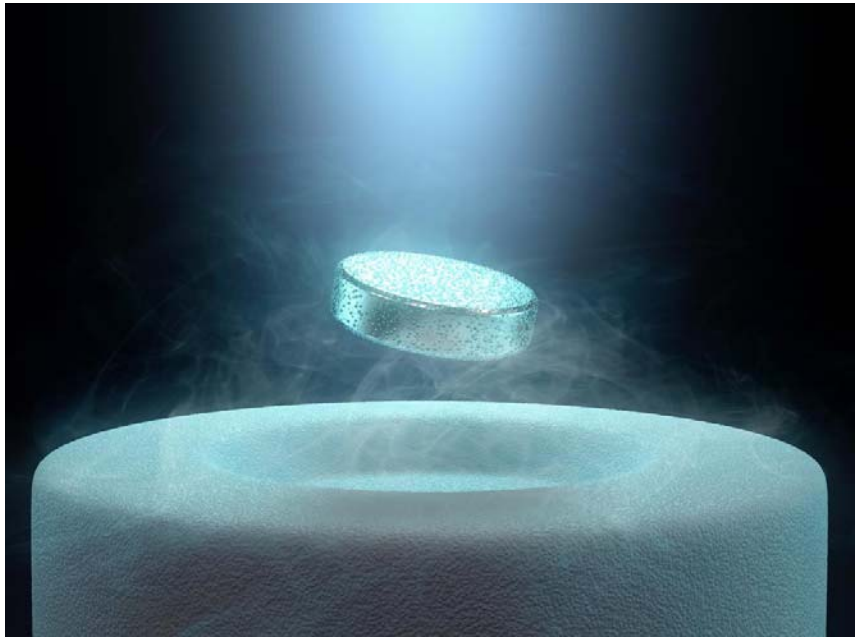
Pump
- ✓ Break Cooper pairs
- ✓ Electrons across band gap
- ✓ Create hot carriers
- ✓ Phonons

Probe
- ✓ Transient reflectivity change

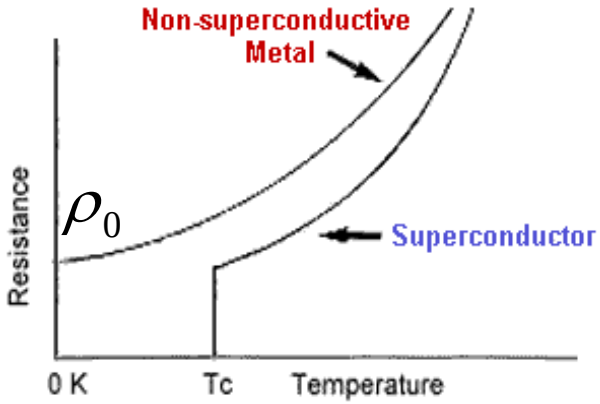
Study
- ✓ Relaxation process

Learn
- ✓ Band structure
- ✓ Gaps
- ✓ Phonons

Fe-based superconductors



Fe-based superconductors

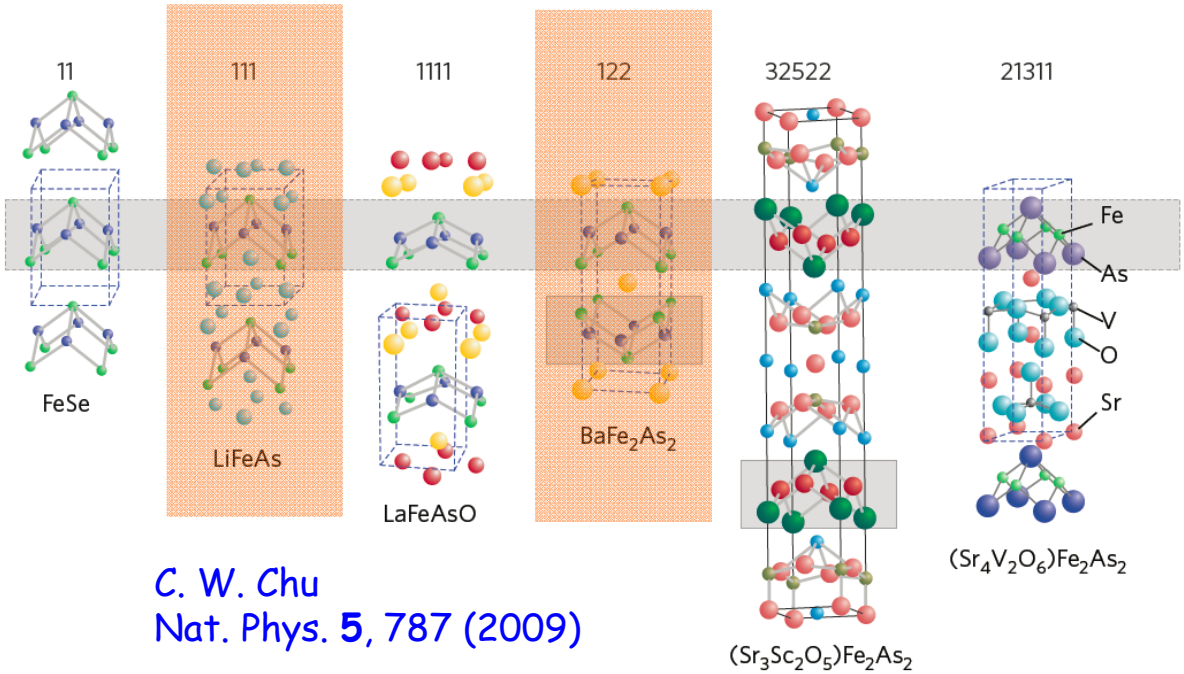


- ✓ Conventional SCs
- ✓ Heavy fermions
- ✓ Cuprates
- ✓ Fe-based SCs

$LaFeAsO_{1-x}F_x$

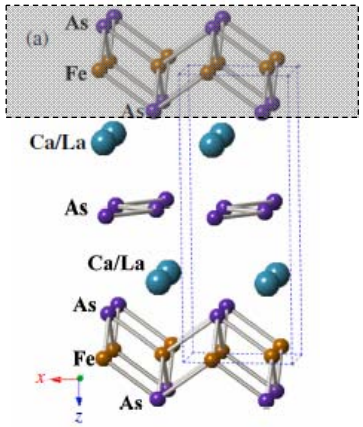
T_c = 26 K

Kamihara *et al.*
JACS **130**, 3296 (2008)



C. W. Chu
Nat. Phys. **5**, 787 (2009)

112

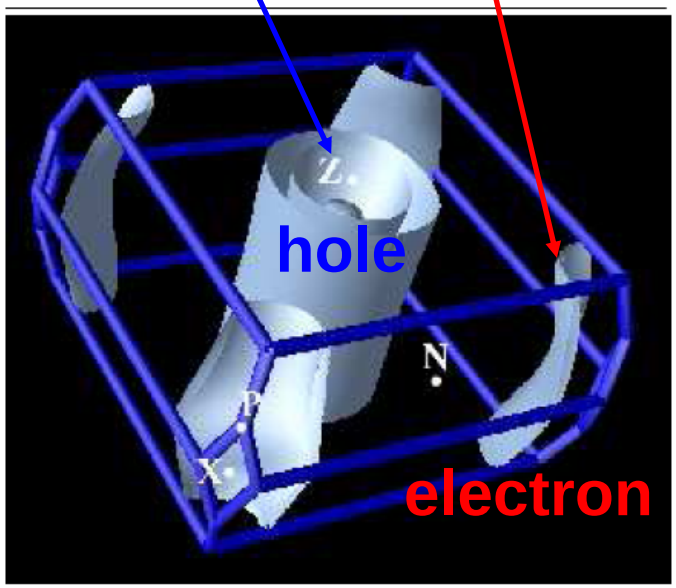


Katayama *et al.*
JPSJ **82**, 123702 (2013)

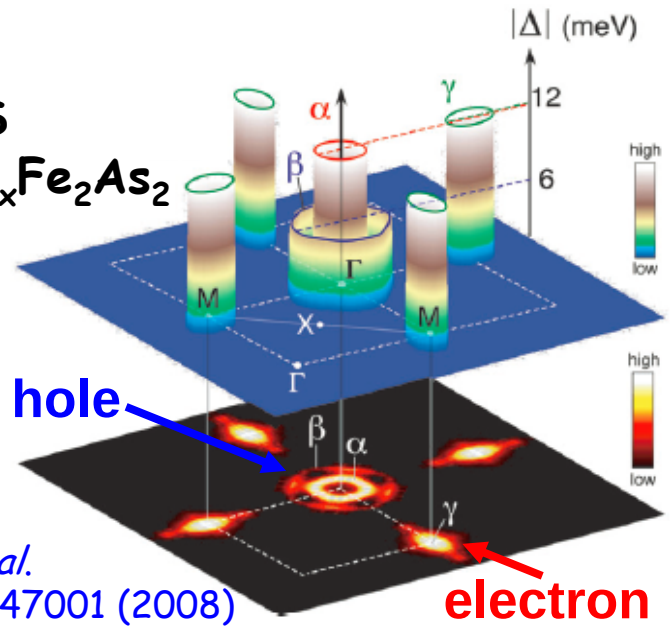
Band structure & Fermi surfaces

M. V. Sadovskii
Phys. Usp. **51**, 1201 (2008)

Multiband materials

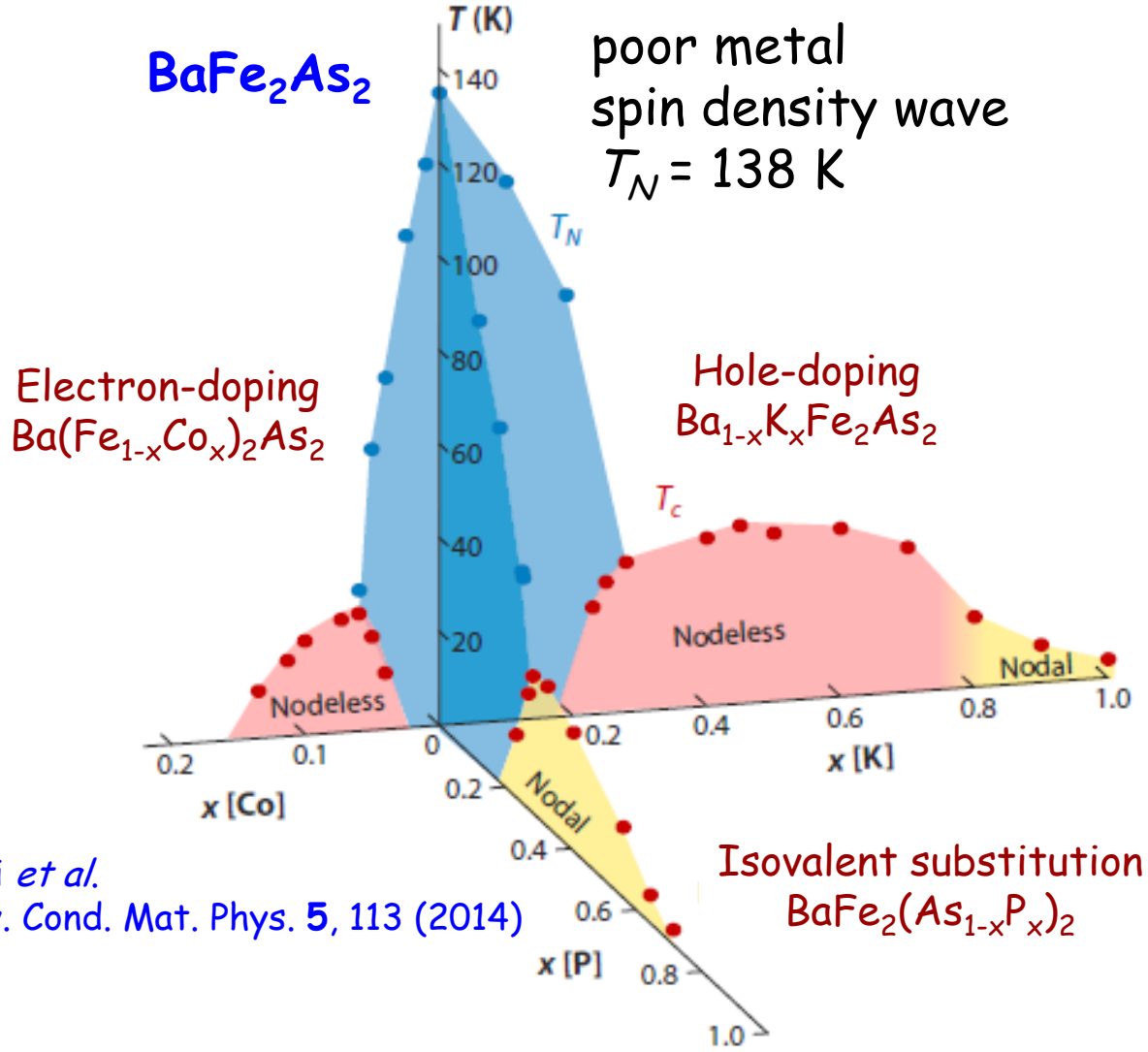


ARPES
$Ba_{1-x}K_xFe_2As_2$



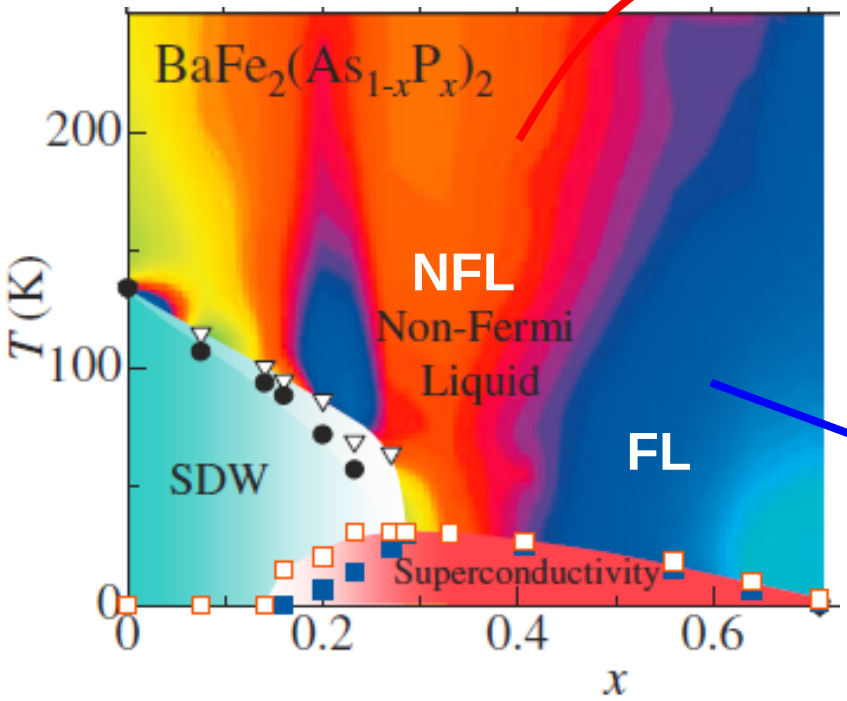
Ding *et al.*
EPL **83**, 47001 (2008)

Ba122 phase diagram

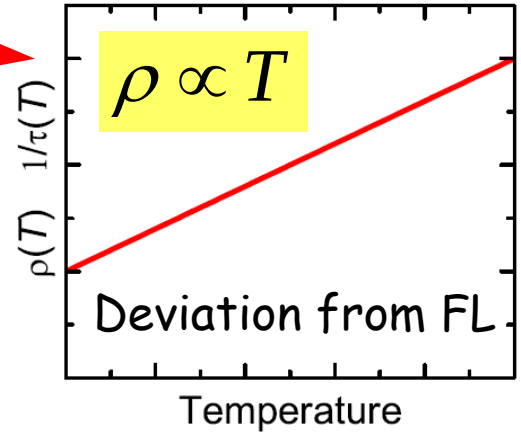


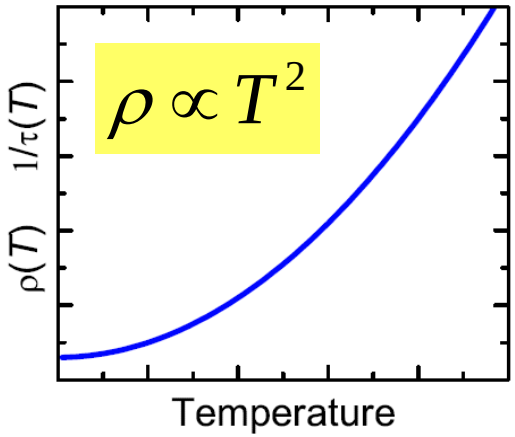
Shibauchi *et al.*
Annu. Rev. Cond. Mat. Phys. **5**, 113 (2014)

Non-Fermi liquid behavior



Kasahara *et al.* PRB **81**, 184519 (2010)

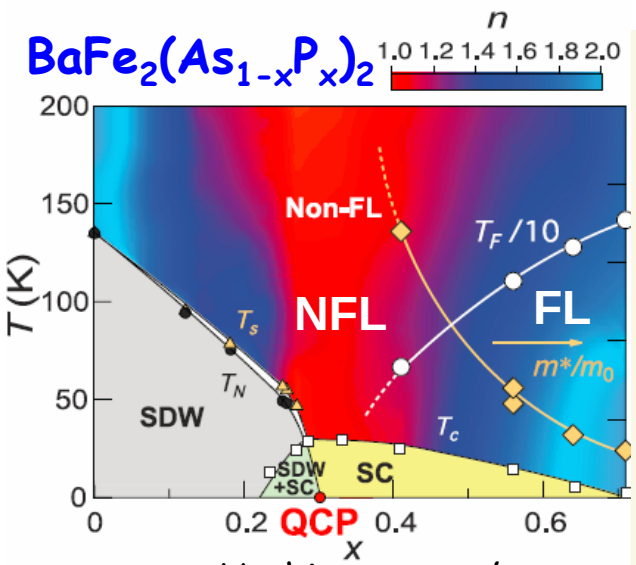




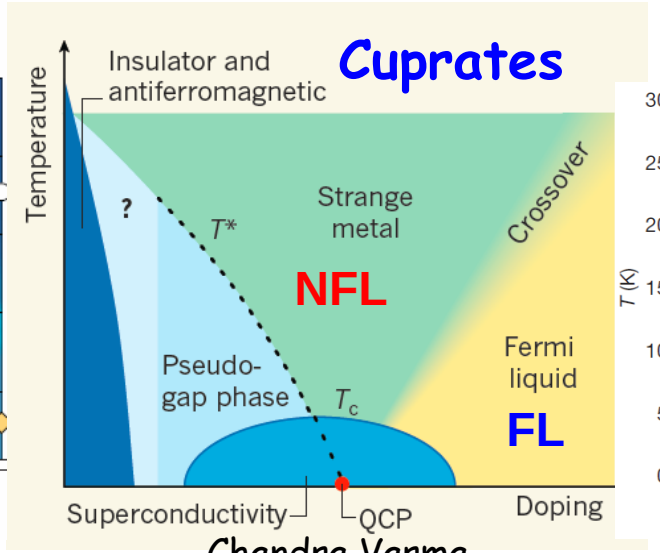
Landau Fermi-liquid theory

Lohneysen *et al.* RMP **79**, 1015 (2007)

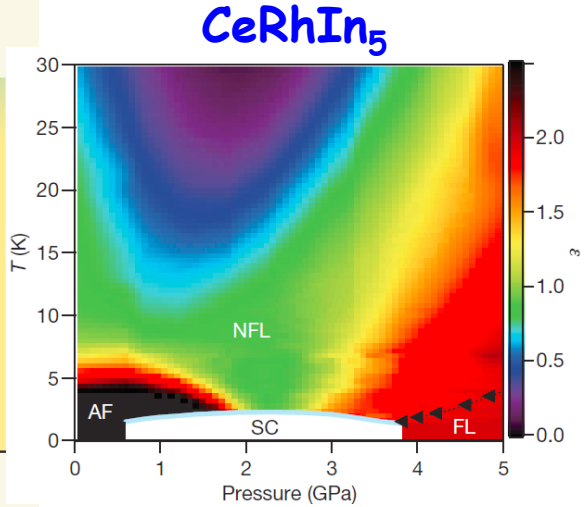
Non-Fermi liquid behavior



Hashimoto *et al.*
Science **336**, 1554 (2012)



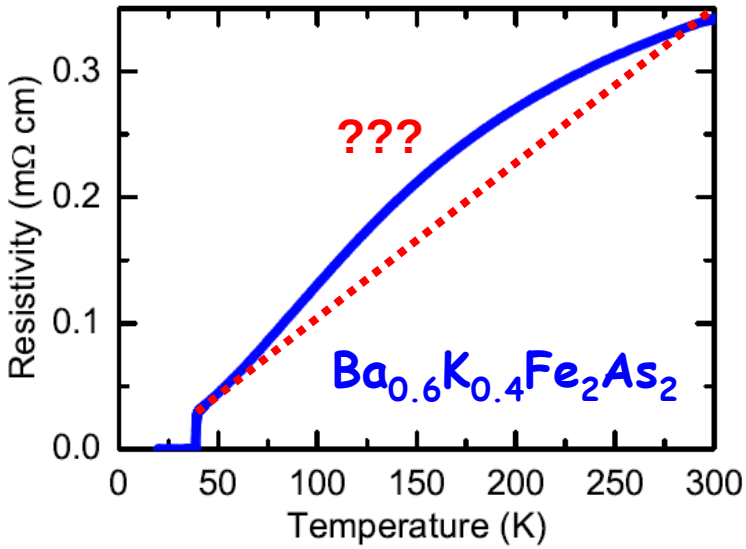
Chandra Varma
Nature **468**, 184 (2010)



Park *et al.*
Nature **456**, 366 (2008)

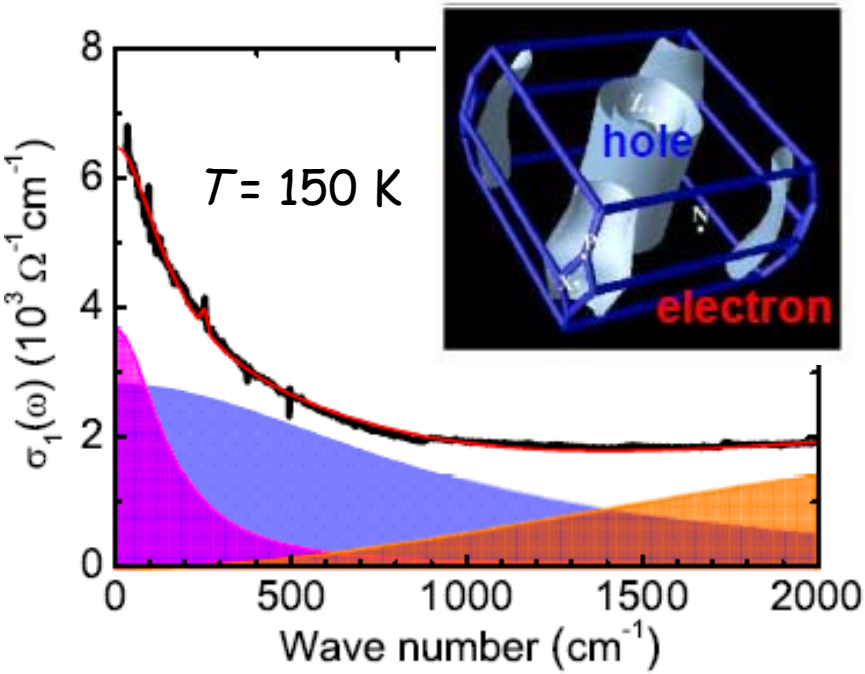
NFL normal state may hold the key to SC!

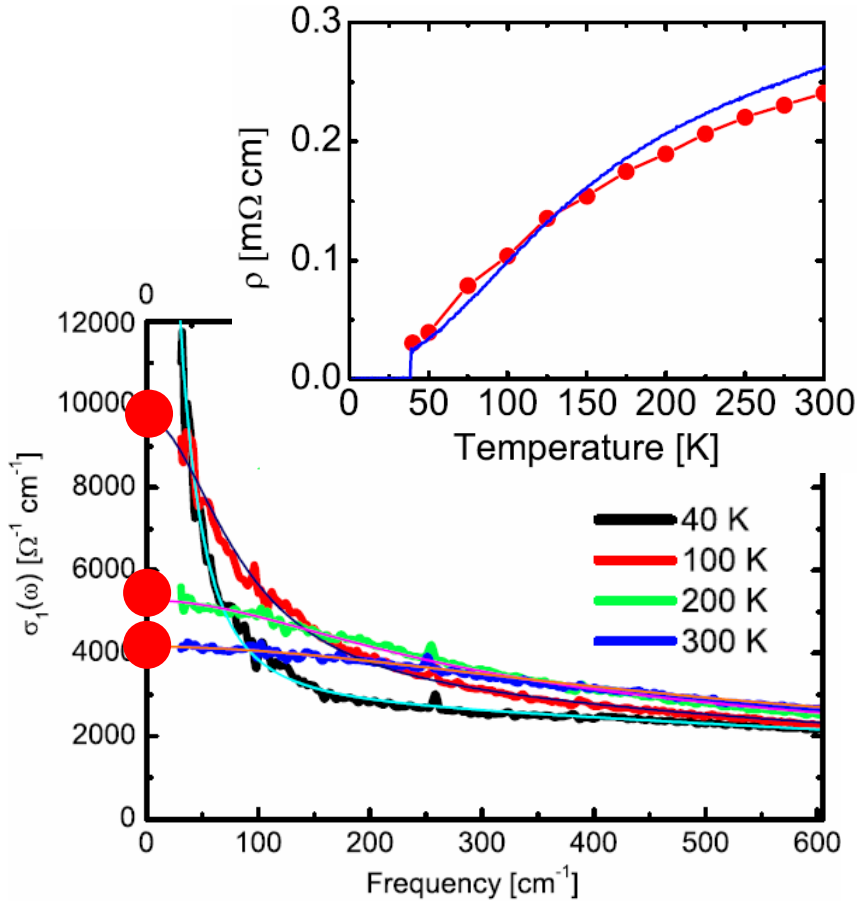
- ✓ NFL common in Fe-based SCs?
- ✓ Mechanism of NFL?
- ✓ Relation between NFL and SC?



Hidden NFL in $Ba_{0.6}K_{0.4}Fe_2As_2$

Dai *et al.* PRL **111**, 117001 (2013)

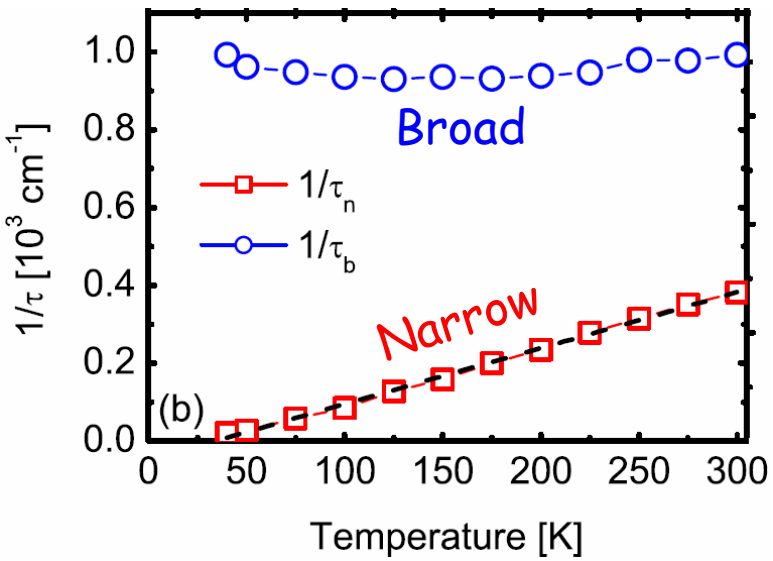




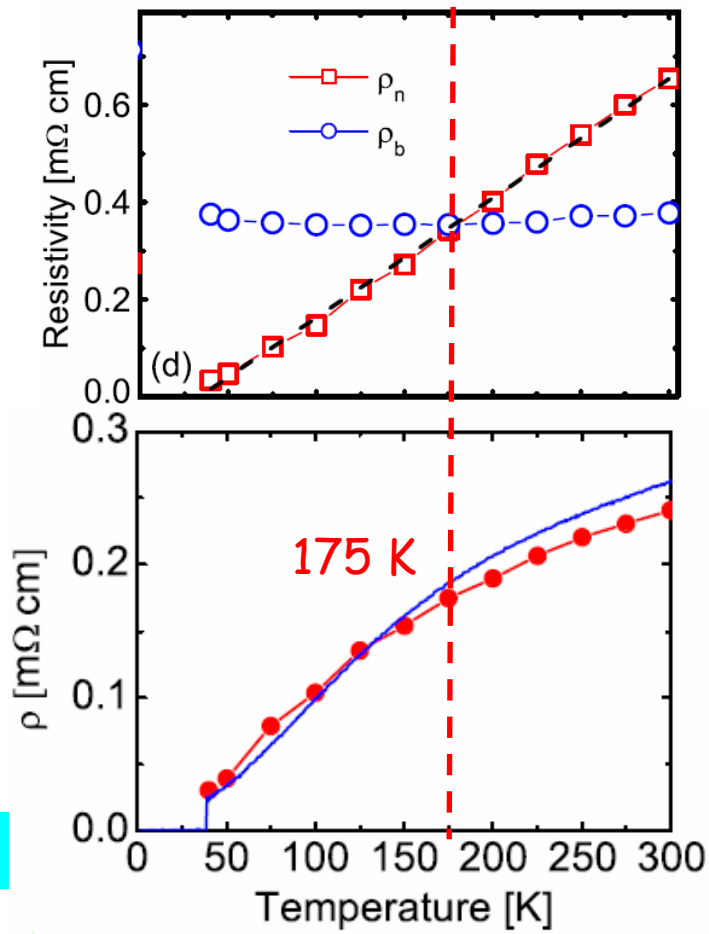
Two Drude components:
narrow & **broad**

Hidden NFL in $Ba_{0.6}K_{0.4}Fe_2As_2$

Dai *et al.* PRL **111**, 117001 (2013)



Parallel circuit: $\sigma_{total} = \sigma_n + \sigma_b$



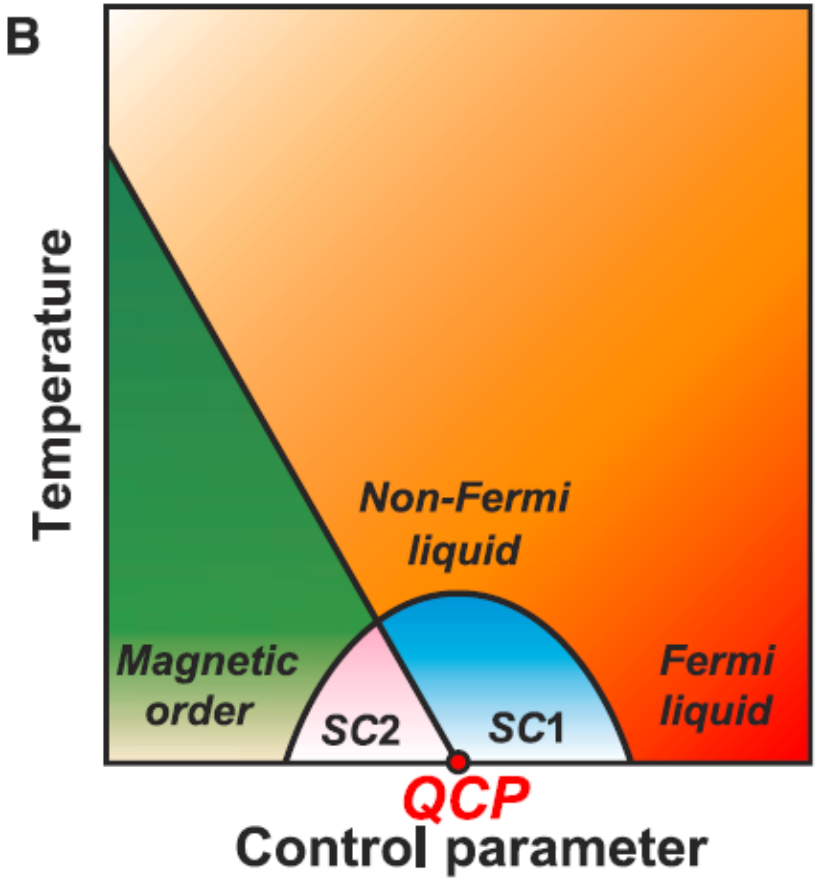
$T < 175$ K $\quad \sigma_n > \sigma_b$ Narrow dominates

$T > 175$ K $\quad \sigma_n < \sigma_b$ Broad dominates

$T = 175$ K $\quad \sigma_n \approx \sigma_b$ Crossover regime

NFL is common in Fe-SCs, but may be hidden

Mechanism of NFL



Hashimoto *et al.*
Science **336**, 1554 (2012)

Quantum critical point (QCP)

- ✓ Ba122 Fe-based SCs
- ✓ Cuprates
- ✓ Heavy fermions

Magnetic order

↓ non-thermal

Zero temperature

↓

QCP

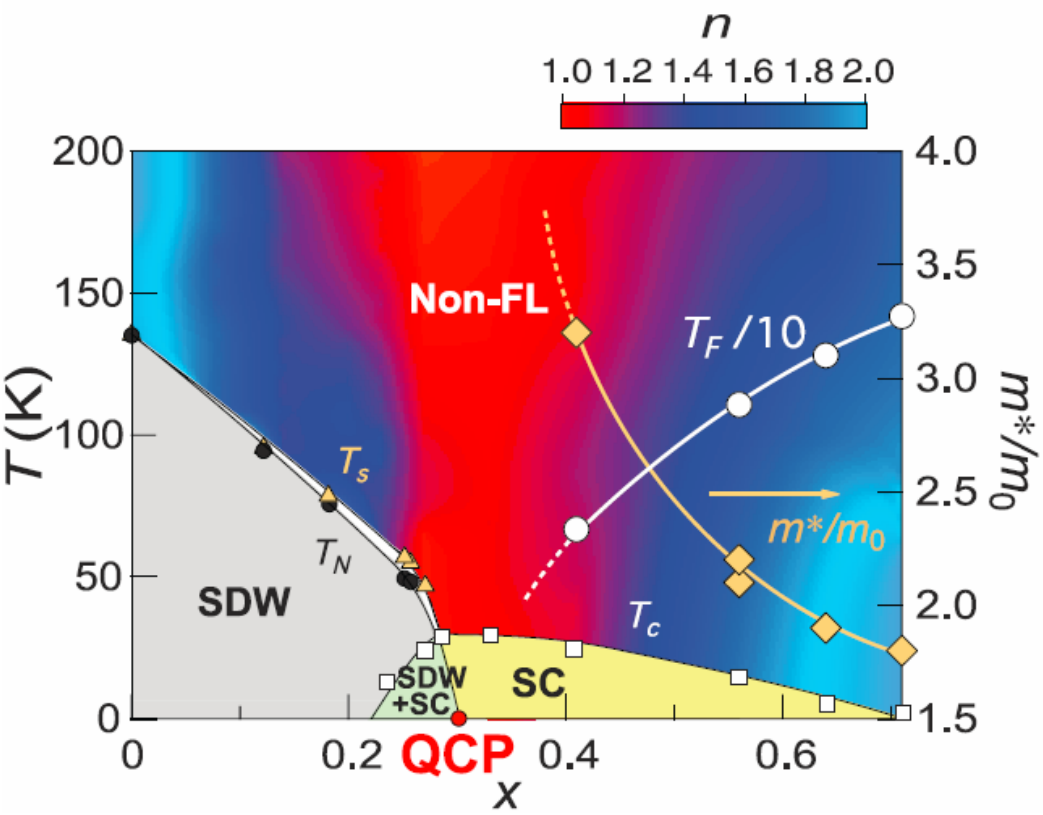
↓

Spin fluctuations

↙ ↘

SC **NFL**

Mechanism of NFL

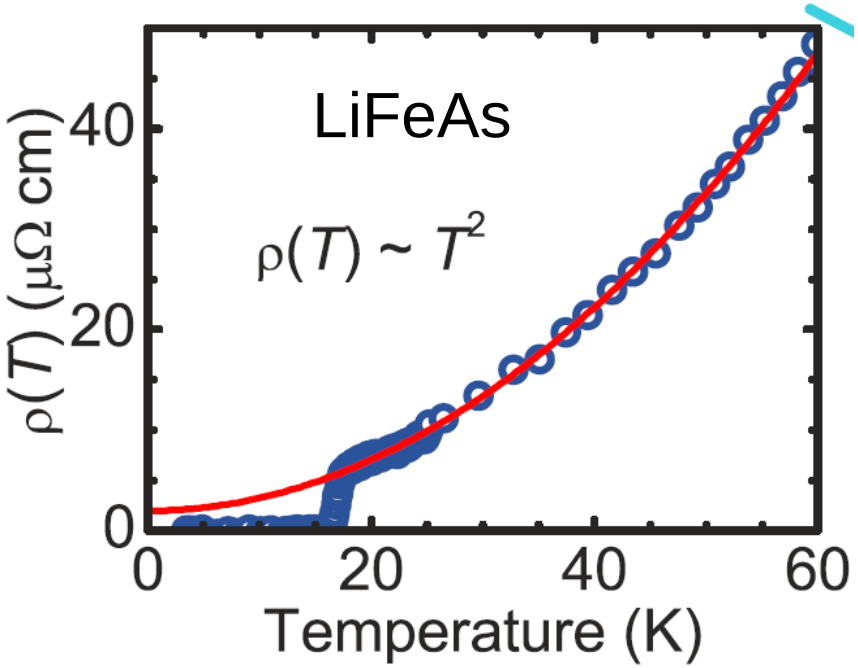


Hashimoto *et al.*
Science **336**, 1554 (2012)

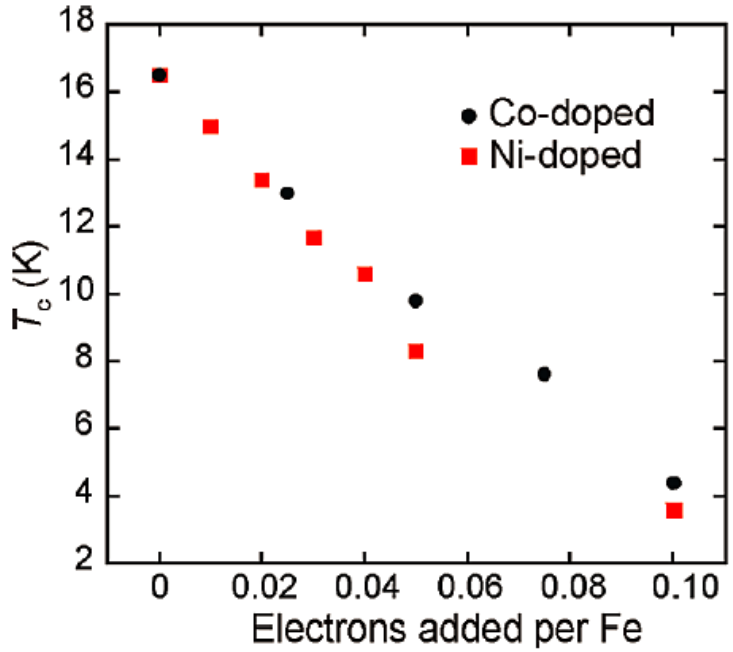
Complicated phase diagram

- ✓ Magnetic order
- ✓ Structural transition
- ✓ Possible QCP(s)
- ✓ Fermi surface nesting
- ✓ Non Fermi liquid
- ✓ Superconductivity

$LiFe_{1-x}Co_xAs$



Dai *et al.* PRB **93**, 054508 (2016)



Pitcher *et al.* JACS **132**, 10467 (2010)

- ✓ SC in stoichiometric form
- ✓ T_c = 18 K
- ✓ Fermi-liquid normal state

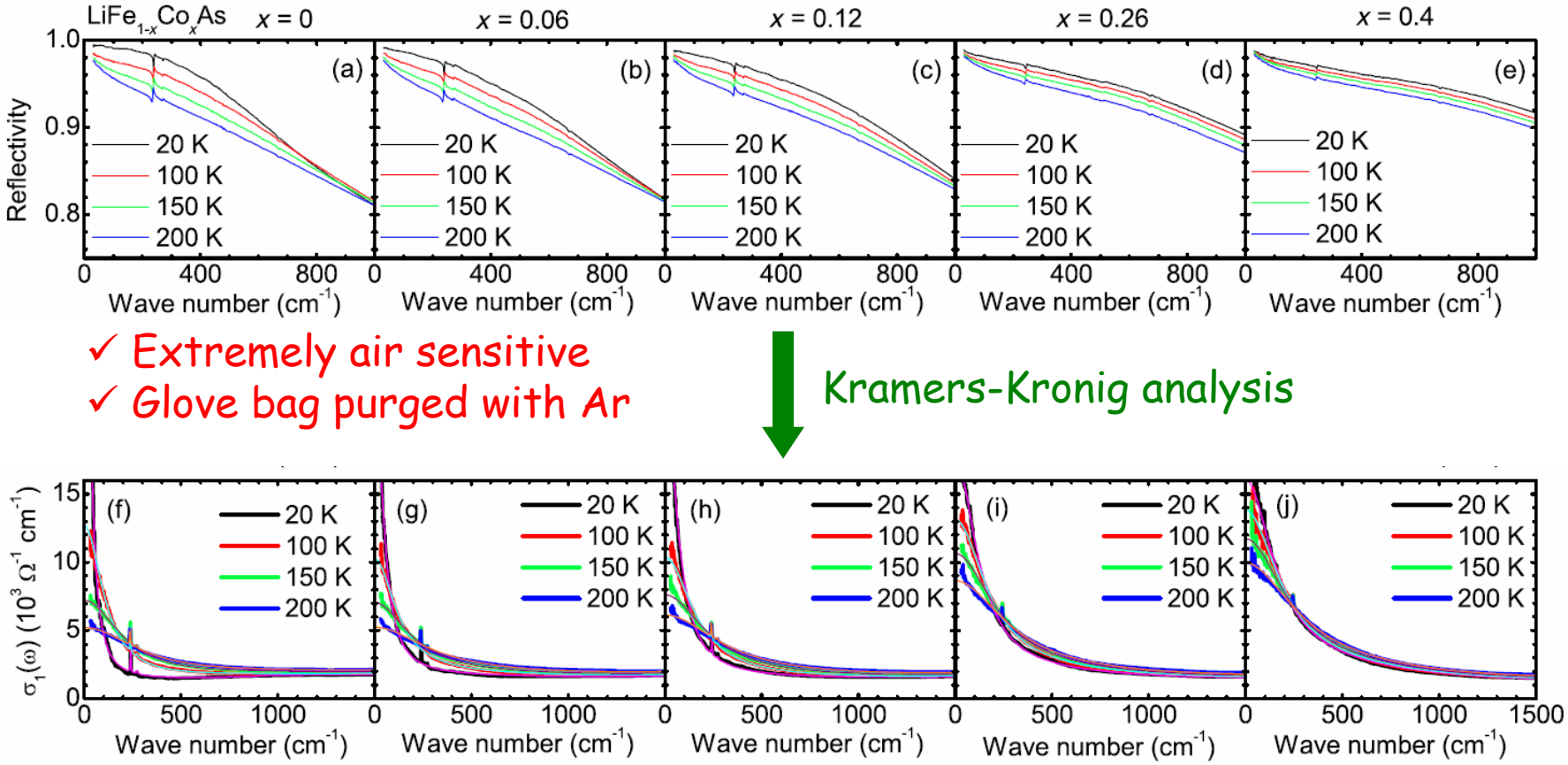
Simple phase diagram

- ✓ No magnetic order
- ✓ No structural transition

FL-NFL-FL crossover in $LiFe_{1-x}Co_xAs$

Reflectivity and optical conductivity

Dai *et al.* PRX **5**, 031035 (2015)



✓ Extremely air sensitive

✓ Glove bag purged with Ar

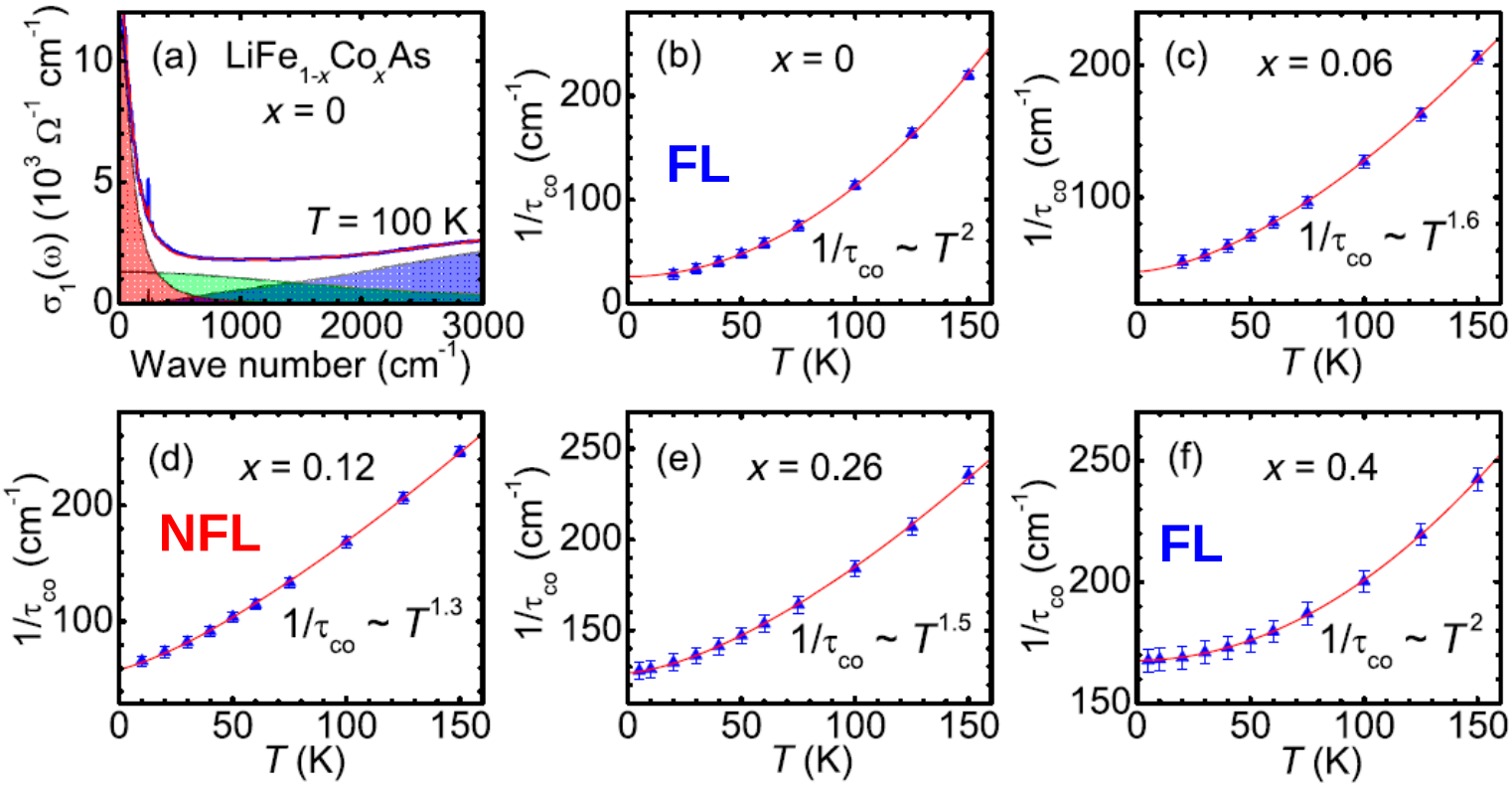
Kramers-Kronig analysis

Pronounced Drude response at low frequencies

FL-NFL-FL crossover in $LiFe_{1-x}Co_xAs$

Scattering rate vs temperature

Dai *et al.* PRX **5**, 031035 (2015)



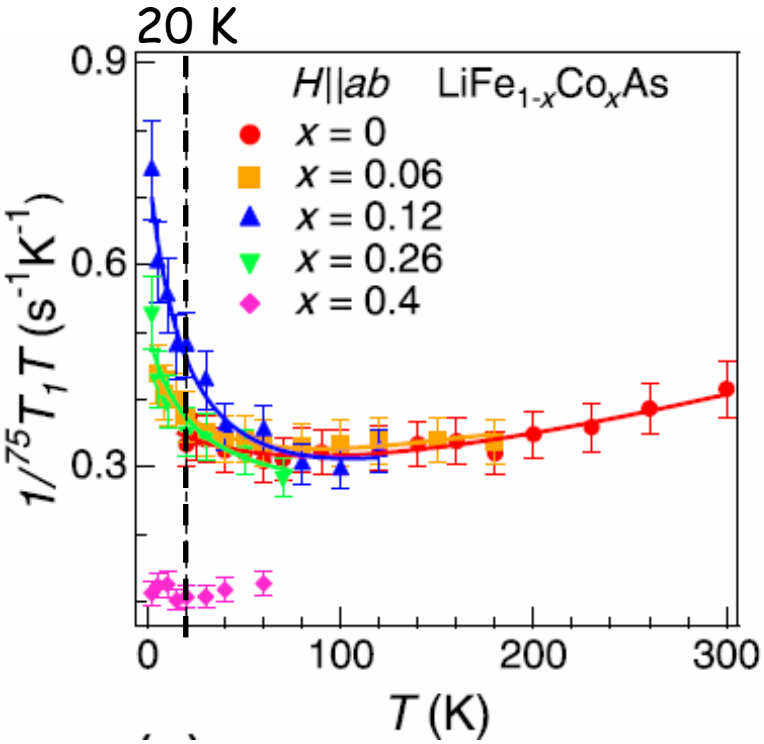
$$1/\tau(T) = 1/\tau_0 + AT^n$$

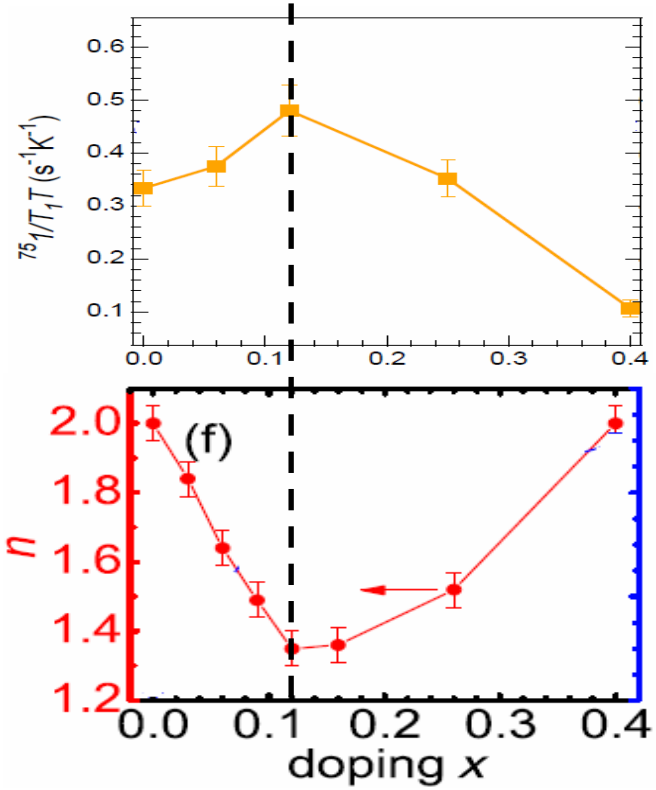
FL-NFL-FL crossover

FL-NFL-FL crossover in $LiFe_{1-x}Co_xAs$

Spin fluctuations? NMR

Dai *et al.* PRX **5**, 031035 (2015)





✓ x = 0: weak T dependence, weak SFs

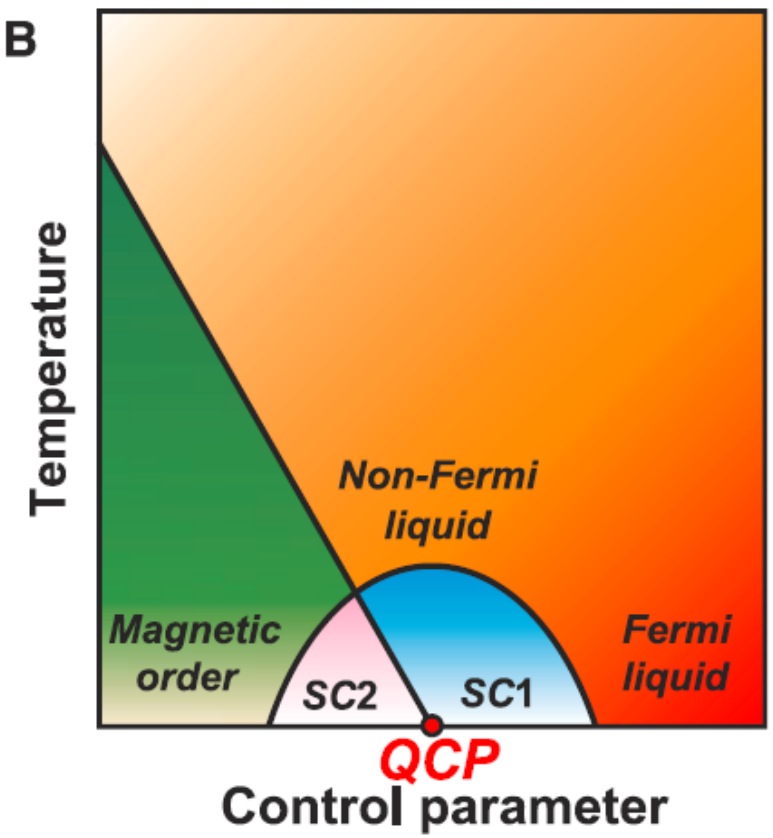
✓ x = 0.12: increase at low T, strong SFs

✓ x = 0.4: weak T dependence, weak SFs

NFL is caused by
Low-energy spin fluctuations

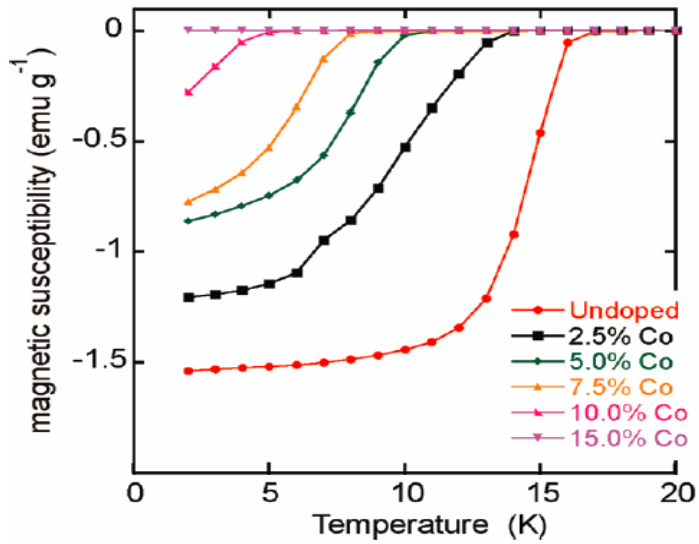
FL-NFL-FL crossover in $LiFe_{1-x}Co_xAs$

Quantum critical point?



Hashimoto *et al.*
Science **336**, 1554 (2012)

Dai *et al.* PRX **5**, 031035 (2015)



Pitcher *et al.* JACS **132**, 10467(2010)

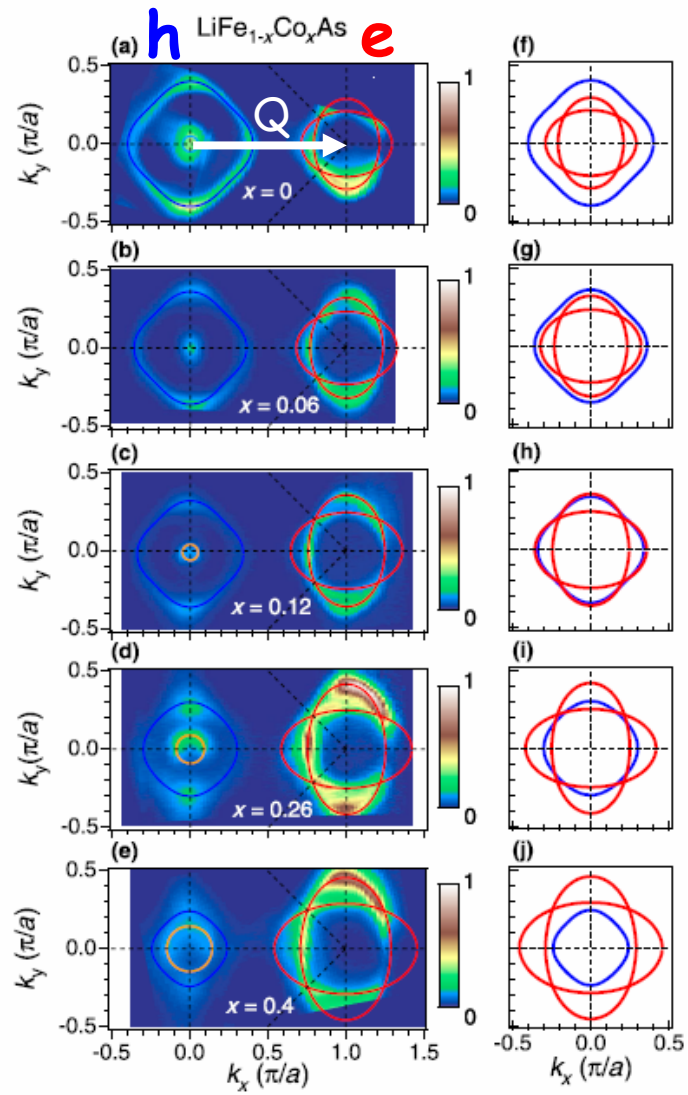
- ✓ Transport
- ✓ Magnetic Susceptibility
- ✓ Infrared spectroscopy
- ✓ ARPES
- ✓ NMR

NO magnetic order up to x = 0.4

FL-NFL-FL crossover in $LiFe_{1-x}Co_xAs$

Fermi surface nesting? ARPES

Dai *et al.* PRX **5**, 031035 (2015)



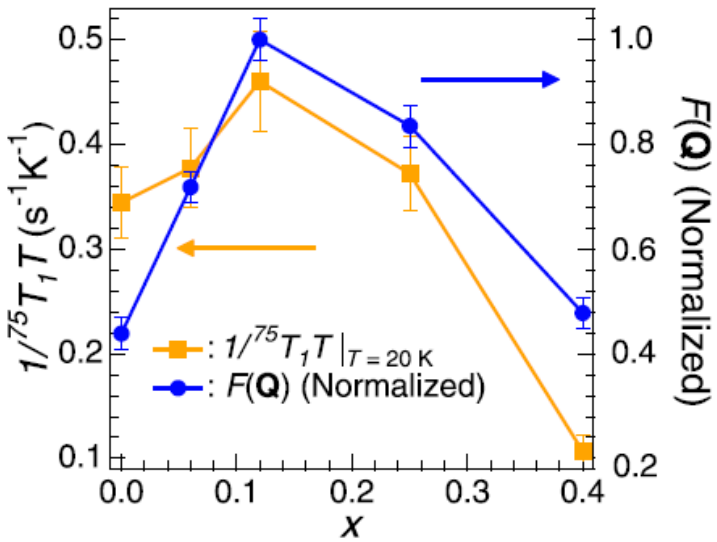
LiFeAs
Poor nesting
Borisenko *et al.*
PRL **105**,067002 (2010)

x = 0.12
perfect
nesting

x = 0.4
poor
nesting

Nesting factor

$$F(\mathbf{Q}) = \sum_{i,j} \int_0^{2\pi} \frac{1}{\|\mathbf{k}_F^{el_i}(\theta) - \mathbf{k}_F^{hole_j}(\theta) - \mathbf{Q}\| + \delta} d\theta,$$

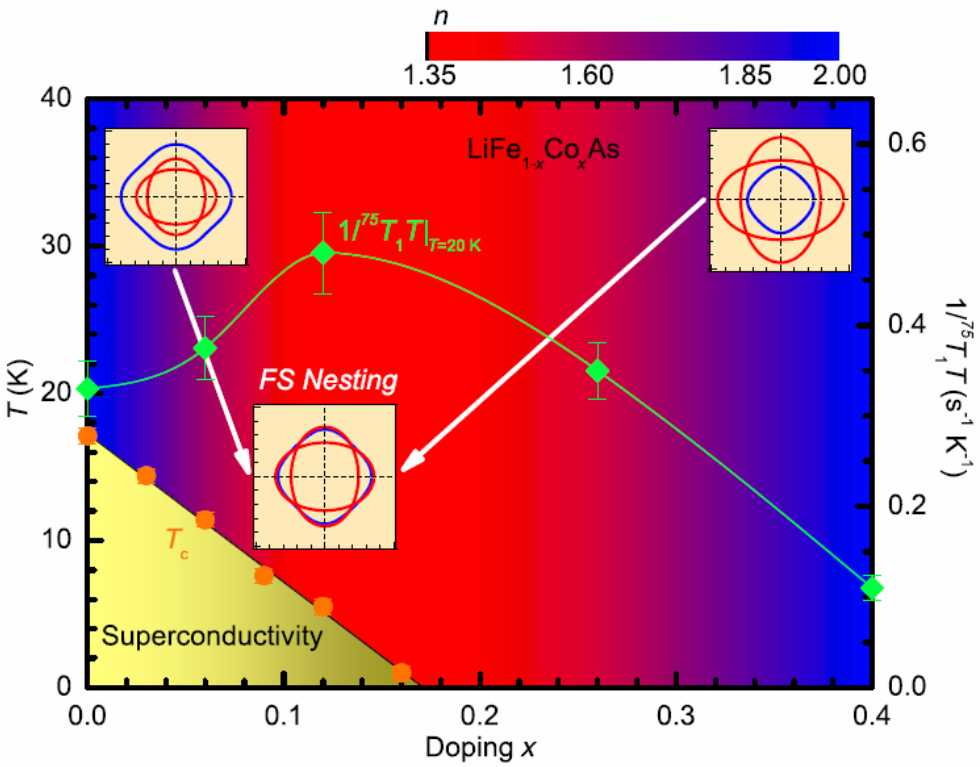


Low-energy spin fluctuations caused by Fermi surface nesting

FL-NFL-FL crossover in $LiFe_{1-x}Co_xAs$

Phase diagram

Dai *et al.* PRX **5**, 031035 (2015)

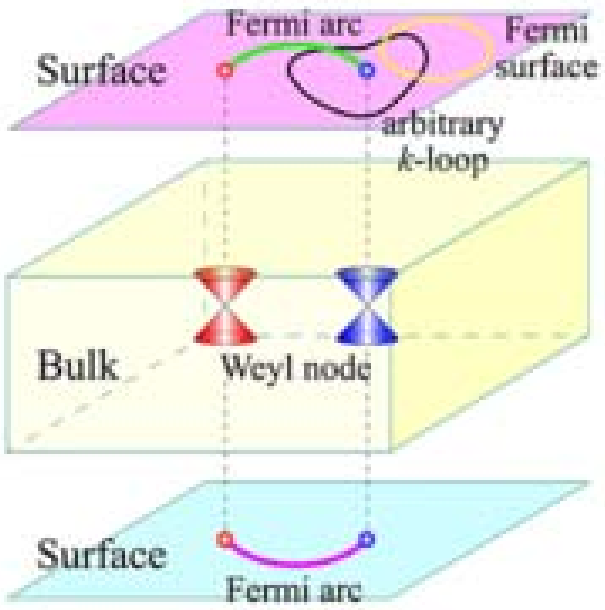


- ✓ FL-NFL-FL crossover
- ✓ NFL caused by Low-energy spin fluctuations (LESFs)
- ✓ LESFs induced by Fermi surface nesting
- ✓ No magnetic order
- ✓ NFL and SC may NOT share the same origin

Further indication: NFL and SC are dominated by spin fluctuations in different energy scales?

Millis, Sachdev & Varma
PRB **37**, 4975 (1988)

Weyl semimetals



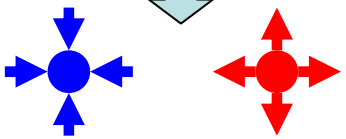
Weyl semimetals

Dirac equation (1928)

Dirac equation *(original)*

$$\left(\beta mc^2 + c\left(\sum_{n=1}^{3} \alpha_n p_n\right)\right)\psi(x,t) = i\hbar\frac{\partial\psi(x,t)}{\partial t}$$

m = 0

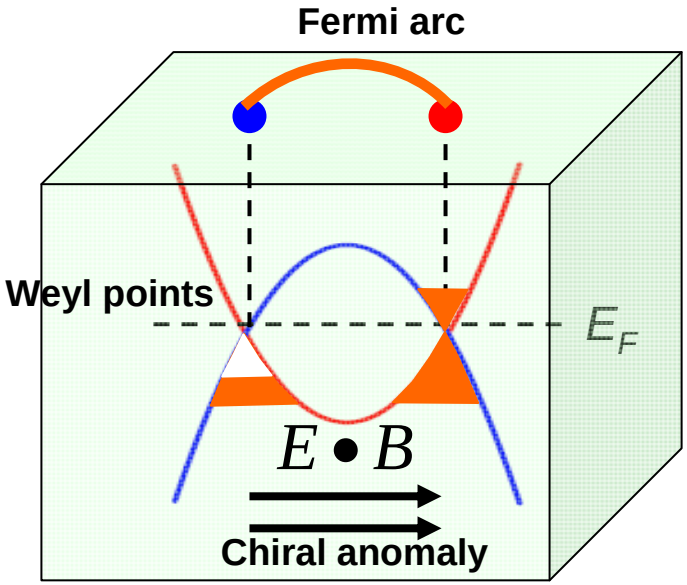


Weyl fermions (1929)

✓ **Exist in high-energy physics ???**

Weyl semimetal (2011)

Wan *et al.* PRB **83**, 205101 (2011)



Materials (2015)

TaAs NbAs TaP NbP WTe_2

Weng *et al*. PRX **5**, 011029 (2015)
Xu *et al*. Science **349**, 613 (2015)
Soluyanov *et al*. Nature **527**, 495 (2015)

Extremely large magnetoresistance (MR)

Ghimire *et al*. JPCM **27**, 152201 (2015)
Huang *et al*. PRX **5**, 031023 (2015)
Ali *et al*. Nature **514**, 205 (2014)

Weyl semimetals

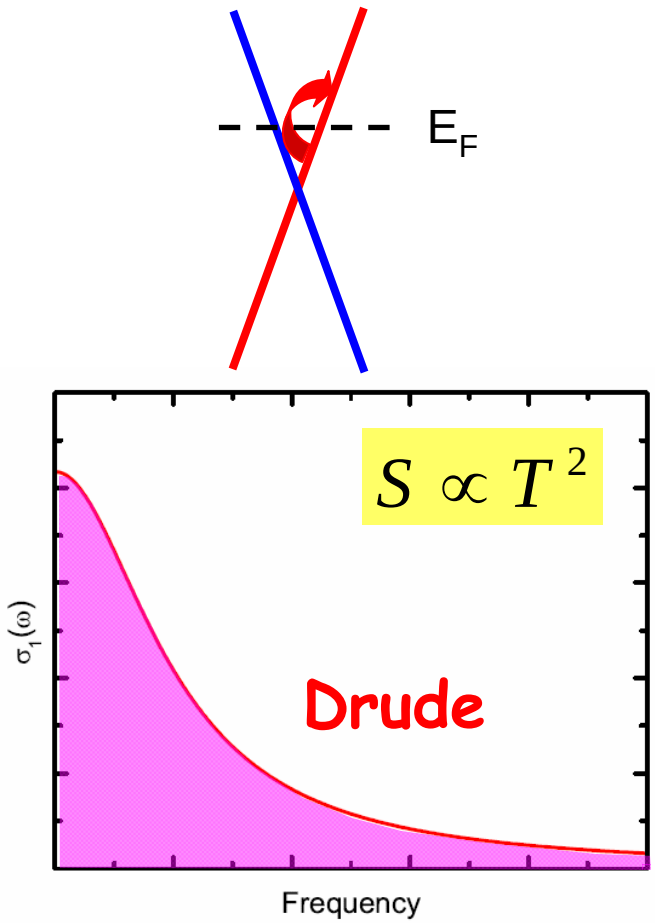
- ✓ Optical signatures of WSMs?
- ✓ Mechanism of the MR?
- ✓ Experimental evidence for the chiral anomaly?
- ✓ Mechanism of the MR sign change?
- ✓ Tunable electron-phonon coupling?
- ✓ Magnetic field-driven Dirac-Weyl transition?
- ✓ Electronic applications?
- ✓ ……

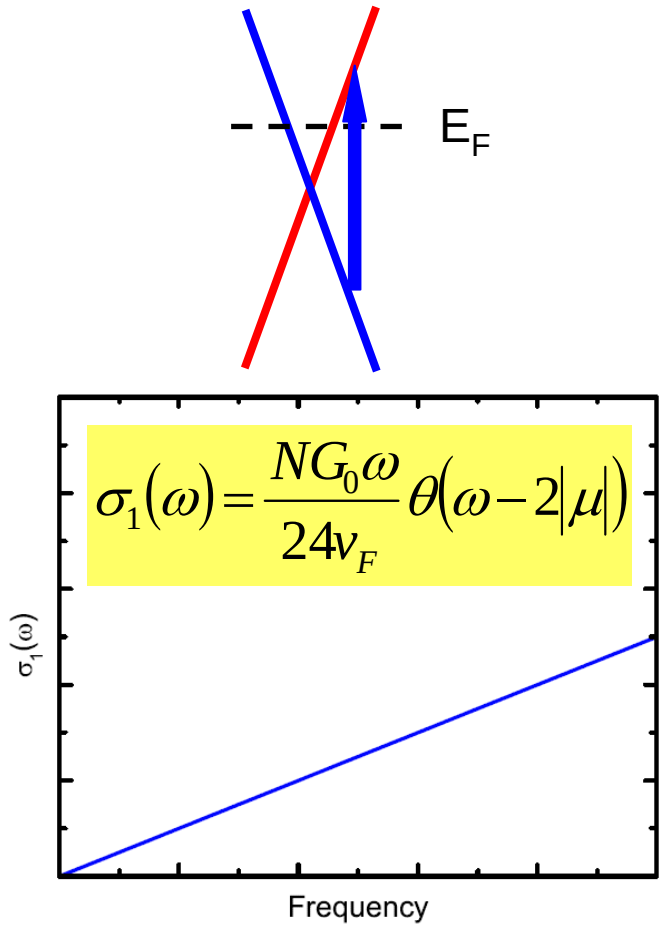
Optical properties of WSMs: Theory

Burkov and Balents PRL **107**, 127205 (2011)
Timusk *et al.* PRB **87**, 235121 (2013)

Hosur *et al.* PRL **108**, 046602 (2012)
Ashby et al. PRB 89, 245121 (2014)

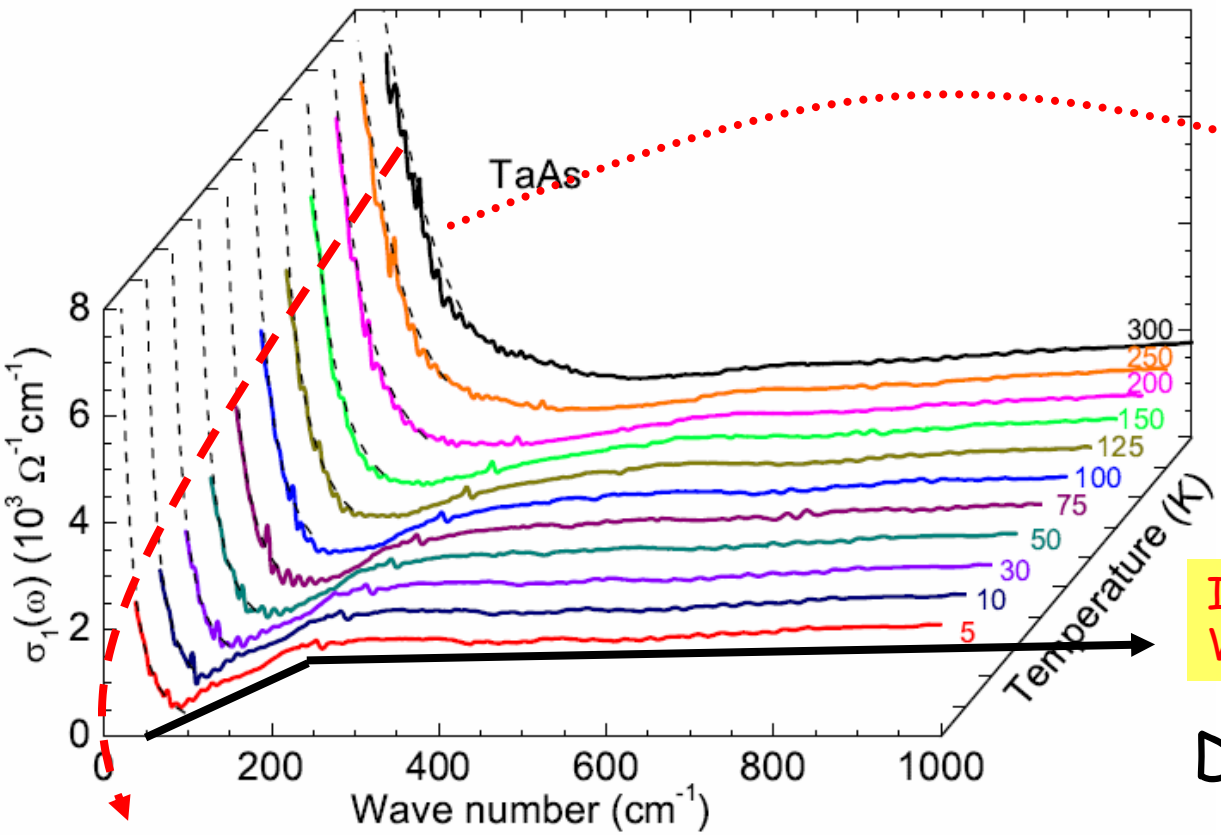
$$\sigma_1(\omega) = \text{Intraband} + \text{Interband}$$





Optical spectroscopy of TaAs

Xu & Dai *et al.* PRB **93**, 121110(R) (2016)



Drude peak

Intraband contribution

Linear conductivity

Interband contribution
Weyl points?

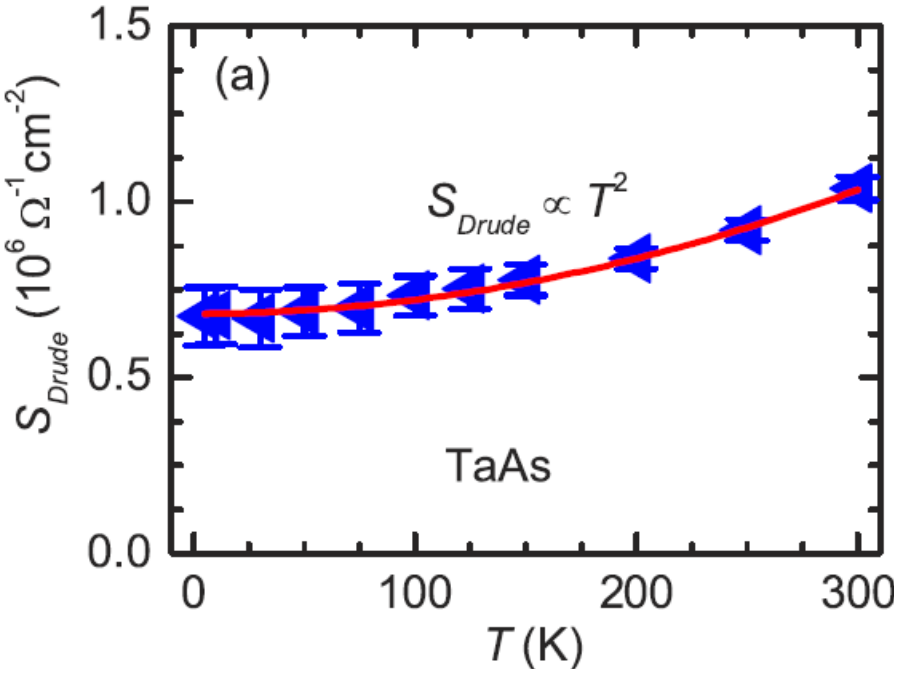
Drude weight decreases with *T*

Drude model

$$\sigma_1(\omega) = \frac{2\pi}{Z_0} \frac{\Omega_p^2}{\tau\left(\omega^2 + \tau^{-2}\right)}$$

Optical spectroscopy of TaAs

Xu & Dai *et al.* PRB **93**, 121110(R) (2016)



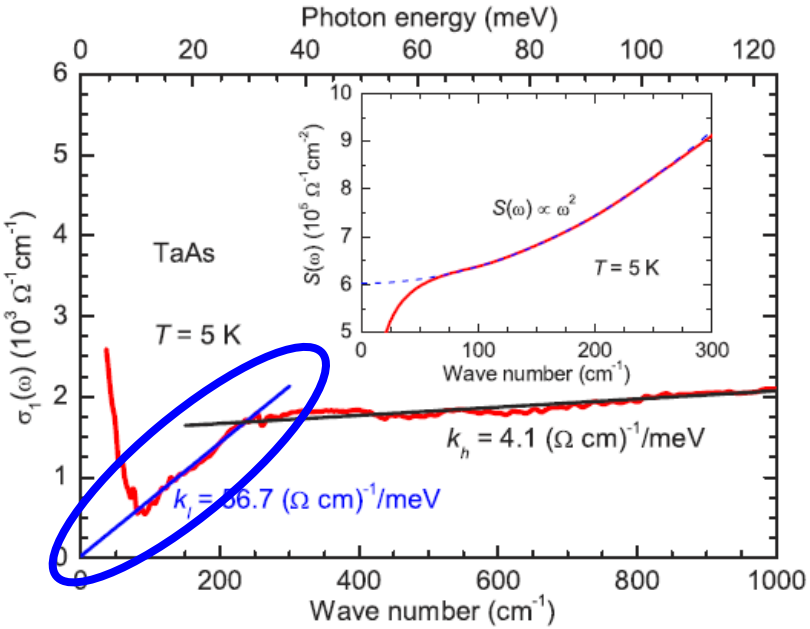
$$S_{Drude} \propto T^2$$

Consistent with theory

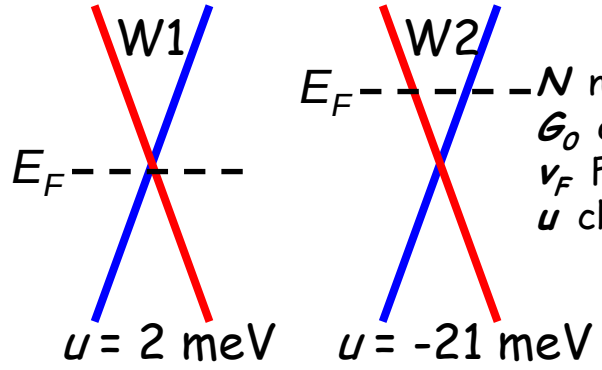
$$S_{\mathrm{Drude}} = \int_0^\infty \sigma_1^D(\omega)d\omega = \frac{\pi^2}{Z_0}\Omega_{p,D}^2.$$

Optical spectroscopy of TaAs

Xu & Dai *et al.* PRB **93**, 121110(R) (2016)



$$\sigma_1(\omega) = \frac{NG_0\omega}{24v_F}\theta(\omega - 2|\mu|)$$



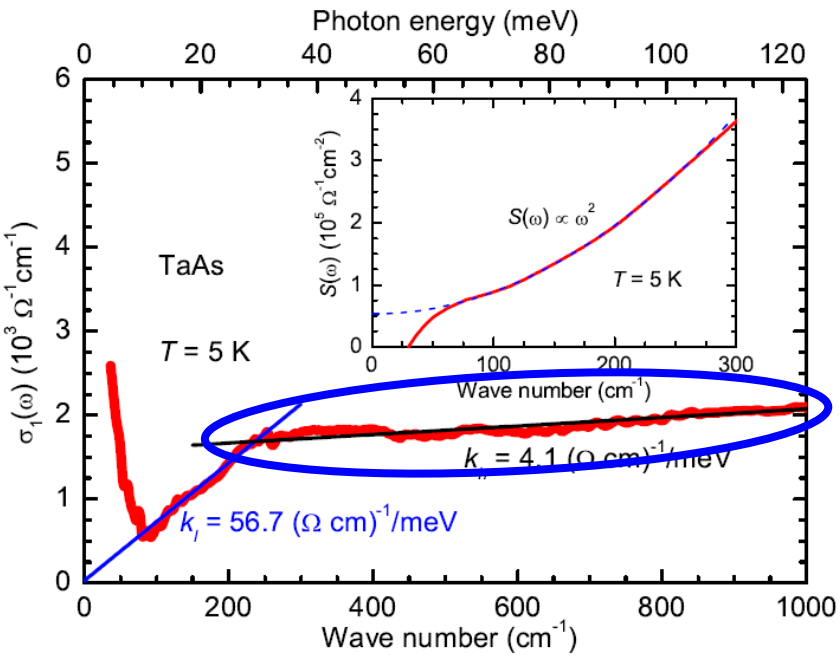
N number of Weyl points
G_0 quantum conductance
v_F Fermi velocity
u chemical potential

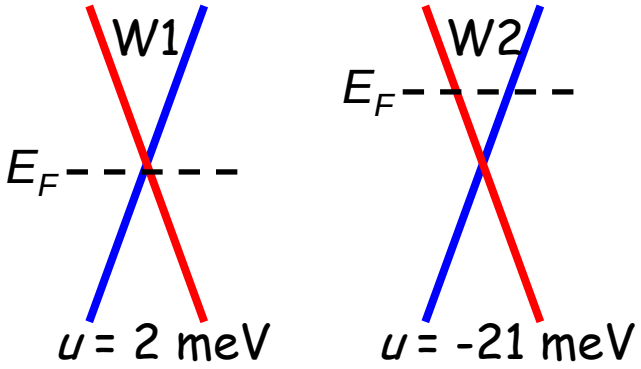
Low-energy linear component:

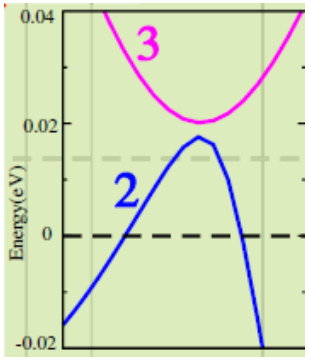
- ✓ Linear in frequency
- ✓ Zero intercept
- ✓ $2|u| < 70$cm^{-1} ($|u| < 4.35$ meV). W2 not turn on until 42 meV (336 cm^{-1})
- ✓ Fermi velocity: for W1, $N = 8$, $v_F = 0.286$ eVA

Optical spectroscopy of TaAs

Xu & Dai *et al.* PRB **93**, 121110(R) (2016)





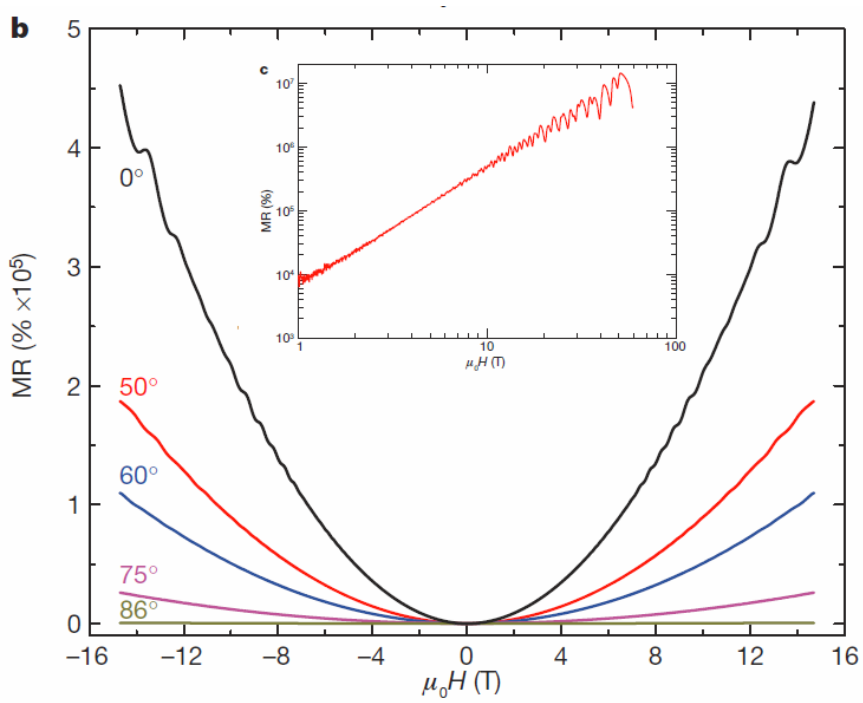


32 cm^{-1} | 336 cm^{-1} | 240 cm^{-1}

High-energy linear component:

✓ Contributions from W1, W2 and trivial bands

Extremely large MR in WTe_2



Ali *et al.* Nature **514**, 205 (2014)

MR = 1.3×10^7% (0.5 K; 60 T)

Application in electronic devices

✓ Magnetic sensors

✓ High-speed hard drives

Electronic cooling: Time scales? Mechanisms?

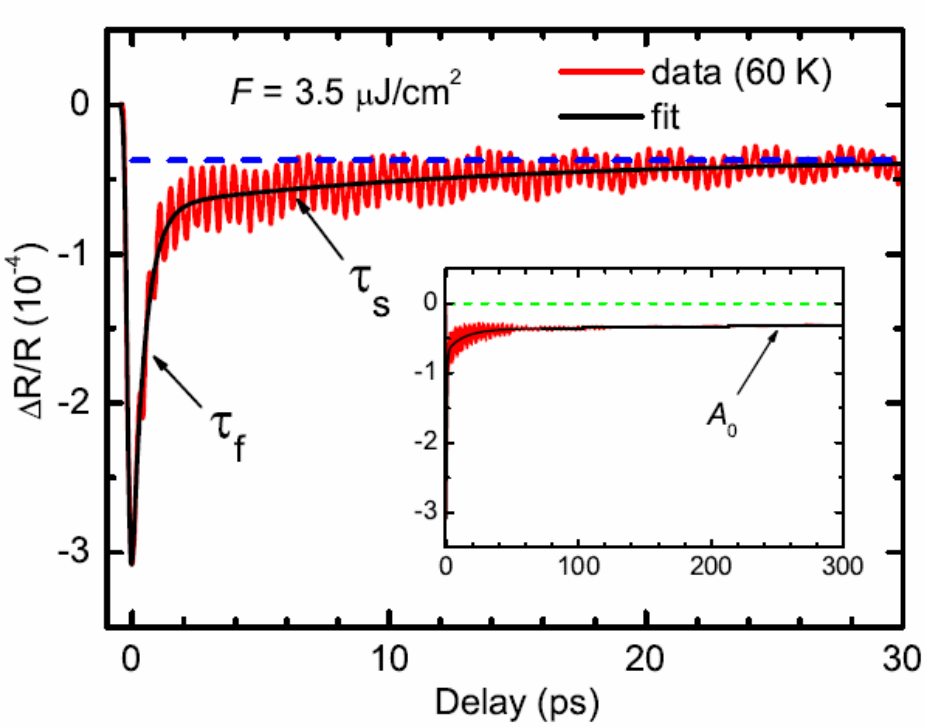
Fundamental physics

✓ Mechanism of large MR

Ultrafast dynamics?

Ultrafast charge dynamics in WTe_2

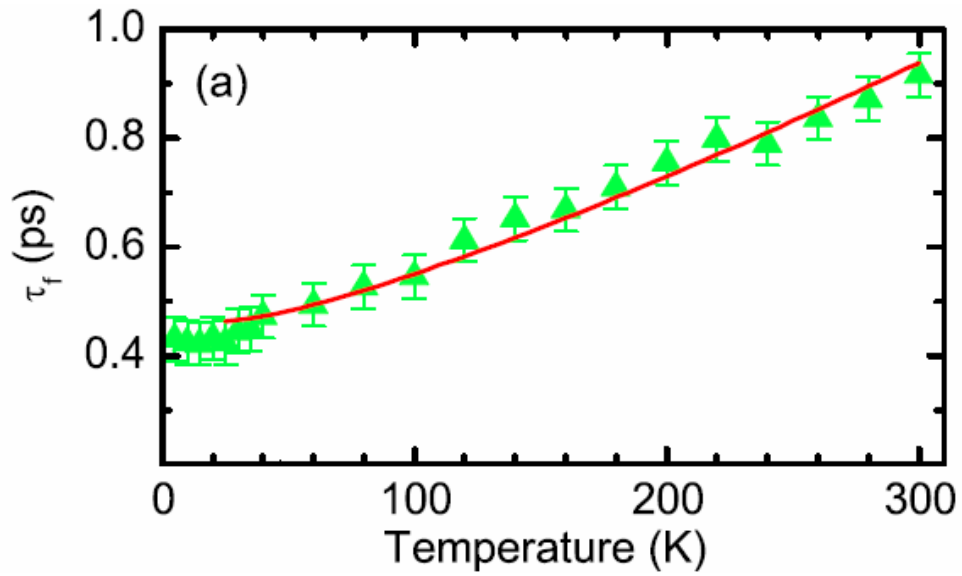
Dai *et al.* PRB **92**, 161104(R) (2015) (Editors' Suggestion)

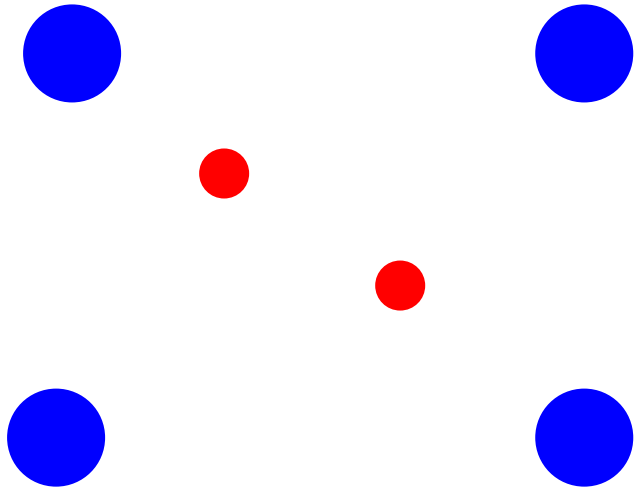


- ✓ Fast decay τ_f **???**
- ✓ Slow decay τ_s **???**
- ✓ Flat offset A_0 Heat diffusion
- ✓ Oscillations Coherent phonons

$$\frac{\Delta R}{R} = A_f e^{-\frac{t}{\tau_f}} + A_s e^{-\frac{t}{\tau_s}} + A_0$$

Ultrafast charge dynamics in WTe_2





$T_e = T_l$

$T_e > T_l$

$T_e \rightarrow T_l$

$T_e = T_l$

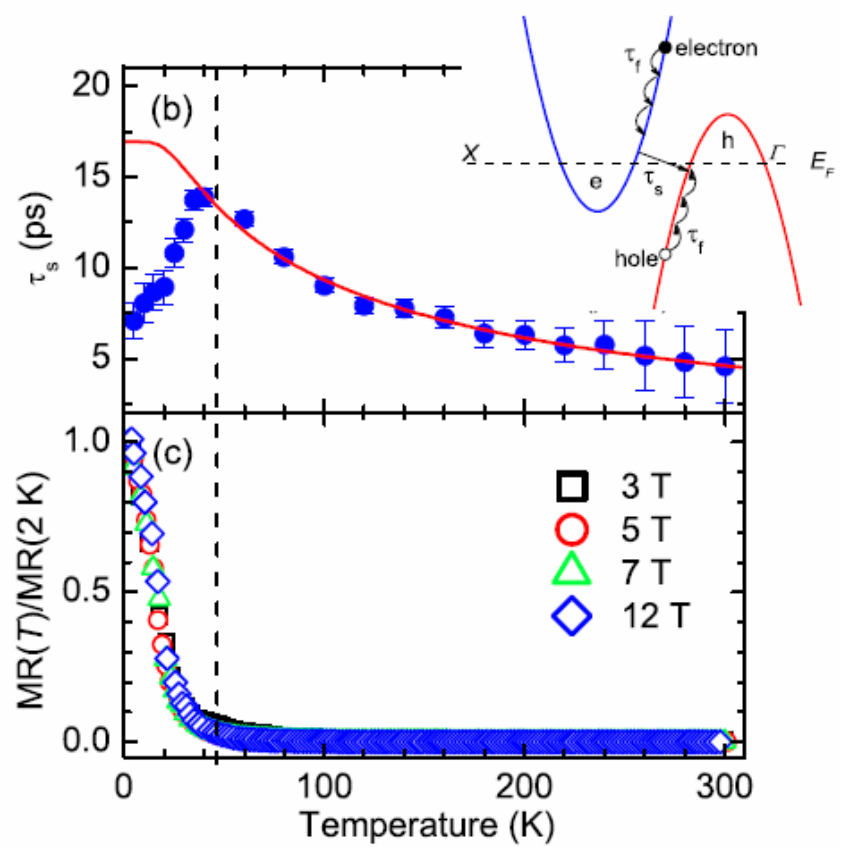
e-ph thermalization
time scale: sub-ps

two temperature model (TTM)

Groeneveld *et al.* PRB **51**, 11433 (1995)
Allen, PRL **59**, 1460 (1987)

Fast decay: e-ph thermalization

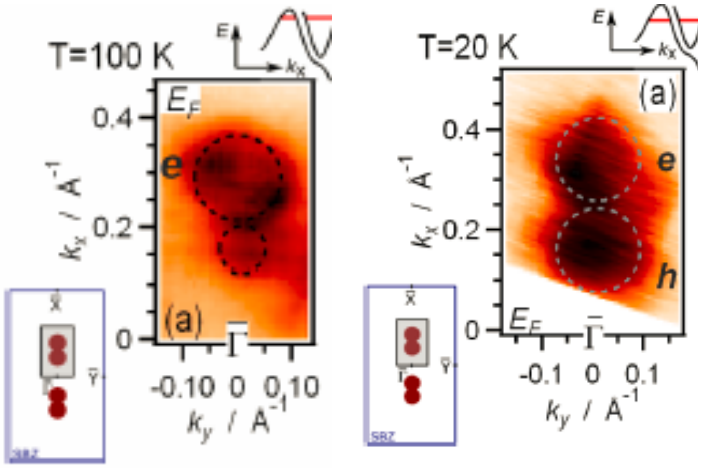
Ultrafast charge dynamics in WTe_2



$$\frac{1}{\tau_R} = A\frac{\frac{\hbar\omega}{2kT}}{\sinh^2\left(\frac{\hbar\omega}{2kT}\right)} + \frac{1}{\tau_I}$$

Lopez, PR **175**, 823 (1968)

- ✓ phonon population
- ✓ joint density of states
- ✓ matrix element



Pletikosic *et al.* PRL **113**, 216601 (2014)

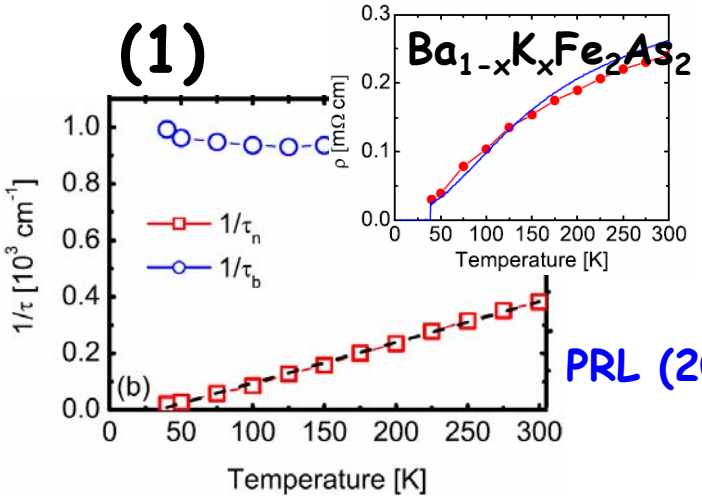
ph-assisted e-h recombination

Bi Lopez, PR **175**, 823 (1968)
Sheu *et al.* PRB **87**, 075429 (2013)

Slow decay ph-assisted e-h recombination; **MR** hole pocket expansion

Summary

(1)

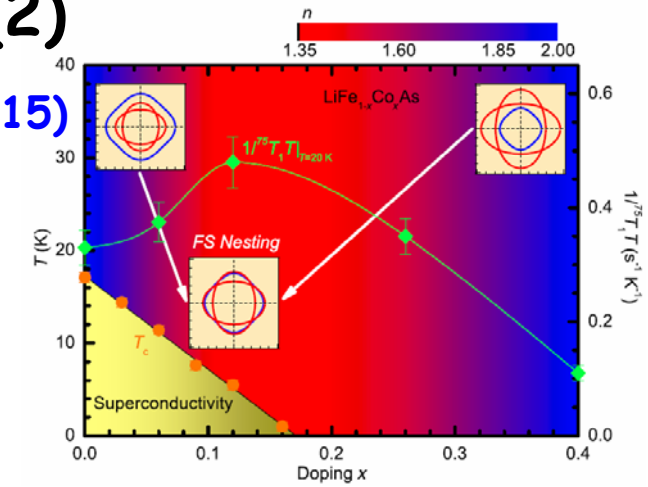


PRL (2013)

Hidden *T*-linear scattering rate (NFL)

(2)

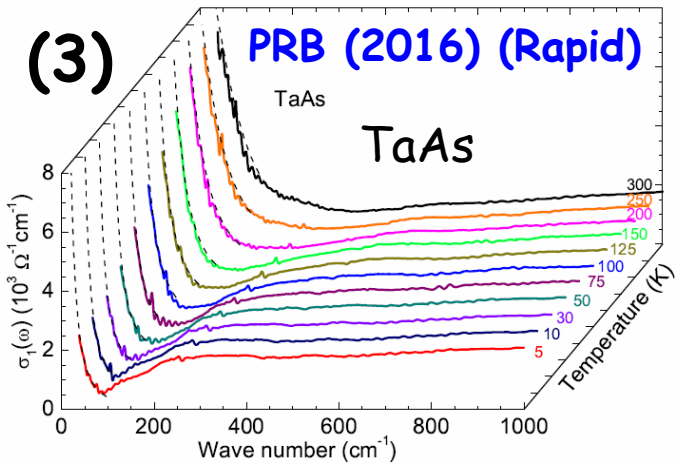
PRX (2015)



- ✓ FL-NFL-FL crossover
- ✓ Low-energy spin fluctuations
- ✓ Fermi surface nesting

(3)

PRB (2016) (Rapid)

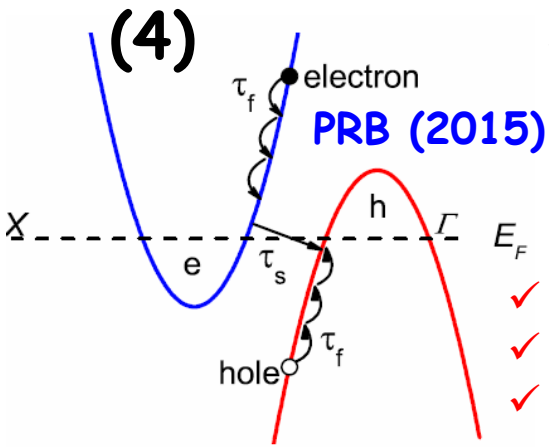


Experiment vs theory

(4)

WTe_2

PRB (2015) (Rapid & Ed. Sug.)



- ✓ e-ph thermalization
- ✓ ph-assisted e-h
- ✓ h pocket expansion

Collaborators

$Ba_{1-x}K_xFe_2As_2$

Sample and transport

B. Shen and H.-H. Wen (NJU, China)

Optics and analysis

Y. M. Dai, B. Xu, H. Xiao, X. G. Qiu, C. C. Homes & R. Lobo (ESPCI, France)

$LiFe_{1-x}Co_xAs$

Sample and transport

L. Y. Xing, X. C. Wang, H. Xiao, X. G. Qiu & C. Q. Jin (IOP CAS, China)

Optics

Y. M. Dai & C. C. Homes (BNL, USA)

ARPES

H. Miao, T. Qian, P. Richard, P. D. Johnson & H. Ding (IOP CAS, China)

NMR

P. S. Wang & W. Q. Yu (Renmin University, China)

Theory

Z. Wang (BC, USA)

TaAs

Sample

L. X. Zhao & G. F. Chen (IOP CAS, China)

Optics

B. Xu, K. Wang, R. Yang, J. Y. Liu, H. Xiao & X. G. Qiu (IOP CAS, China)

Y. M. Dai, A. J. Taylor, D. A. Yarotski & R. P. Prasankumar (LANL, USA)

WTe_2

Sample

H. Li & Y. G. Shi (IOP CAS, China)

Optics

Y. M. Dai, J. Bowlan, A. J. Taylor, D. A. Yarotski & R. P. Prasankumar (LANL, USA)

Thanks!