

# Detection of novel electronic order in Fe-based superconducting (and related) materials with point contact spectroscopy

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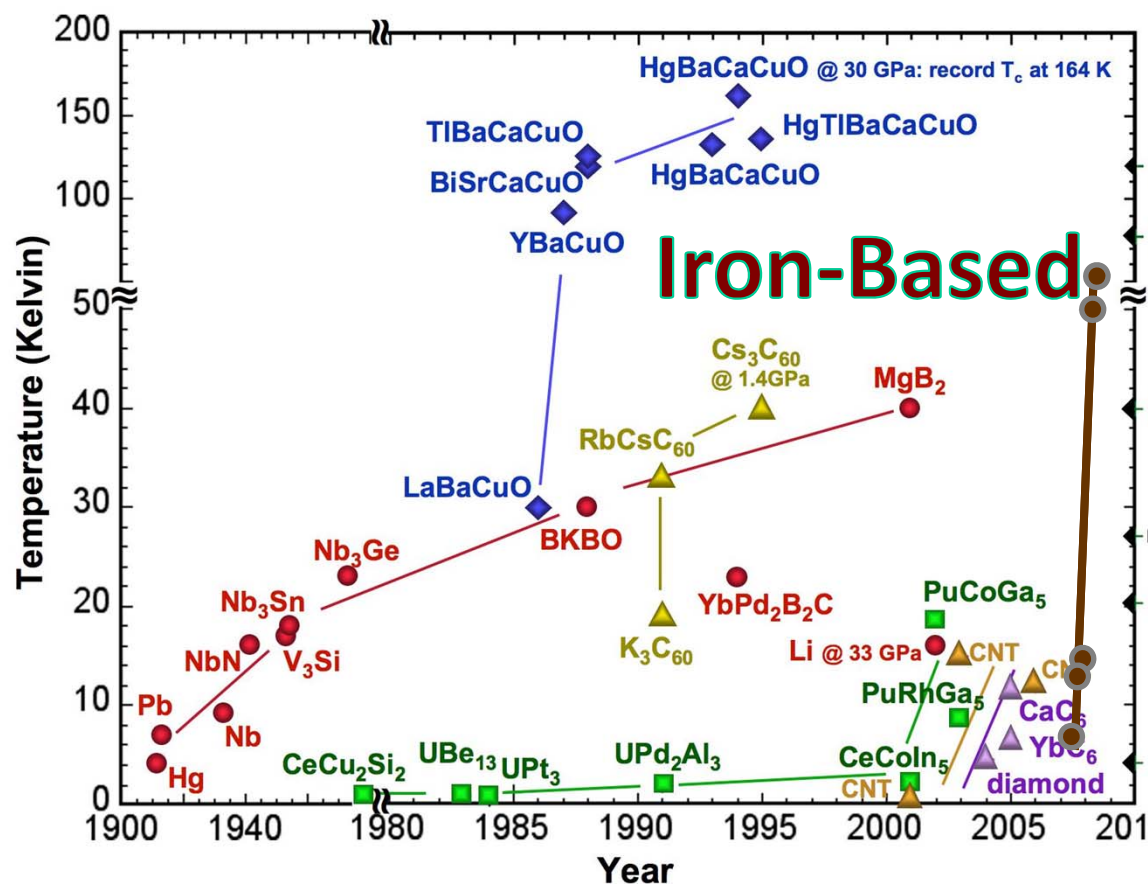


**ICMT Conference on Disordered Materials**

**May 17, 2011**

# After a couple of decades...

## HTS is NOT UNIQUE to Cuprates!!!

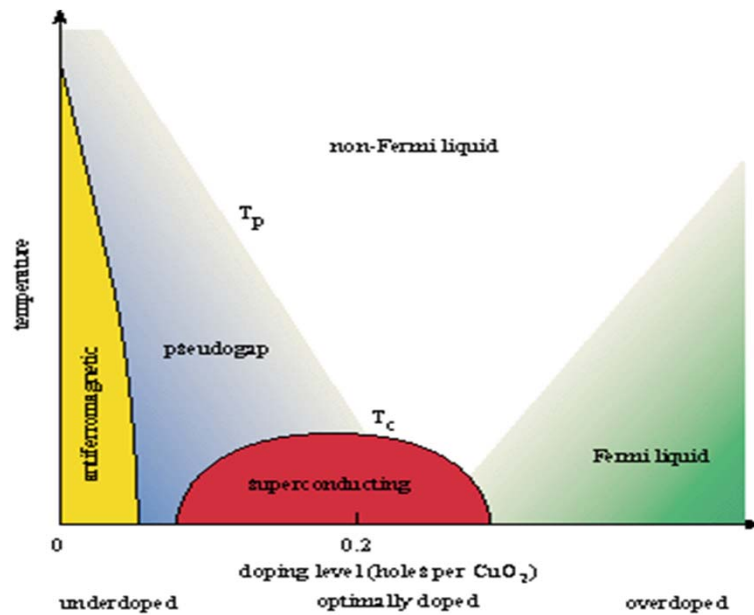


And we still do not understand the mechanism of SC in any of the HTS and related novel superconductors!

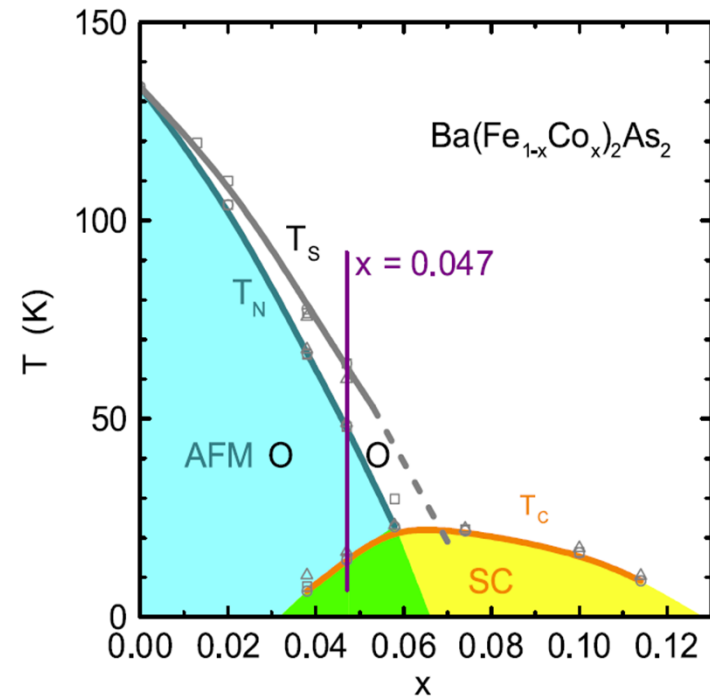
# Generic HTS phase diagrams

## Pressure and doping tuning

### Cuprates



### Fe-Based



# Similar phase diagrams of related materials organic and heavy-Fermion SCs

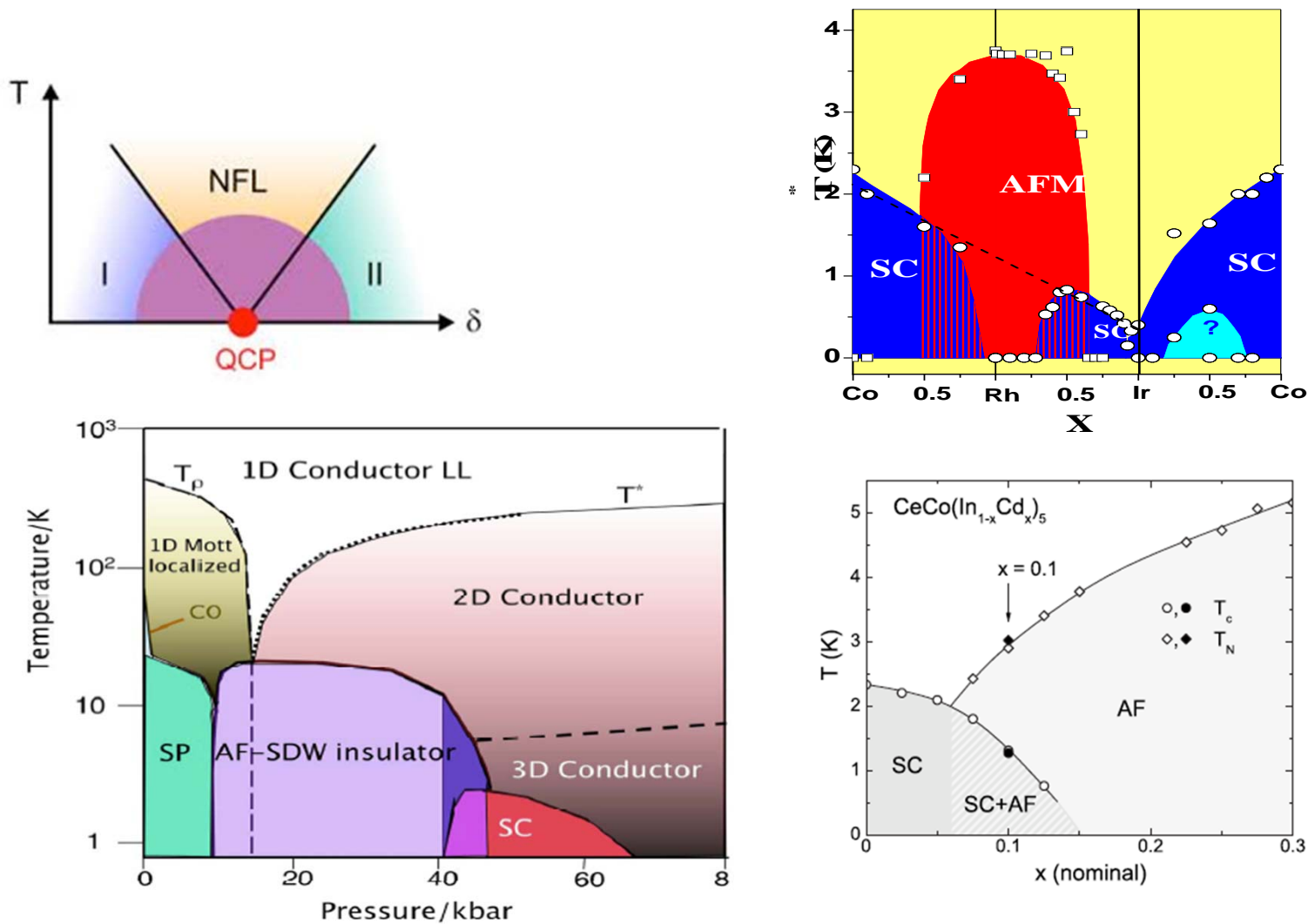


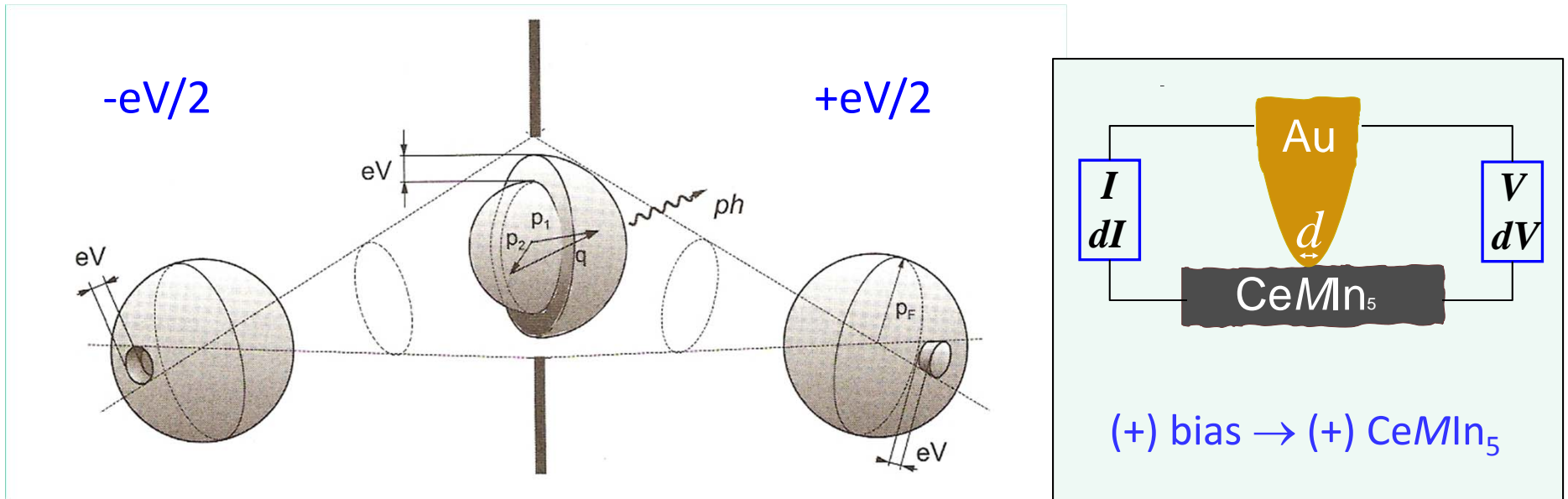
Figure 1: Generic temperature-pressure phase diagram of the  $(\text{TM})_2\text{X}$  family of organic conductors. The diagram is drawn for the compound

# Outline

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- Quasiparticle Scattering Spectroscopy  
[Point-Contact Spectroscopy]
- Heavy Fermion CeCoIn<sub>5</sub>  
Detecting phase orderings and broken symmetries
- Heavy Fermion URu<sub>2</sub>Si<sub>2</sub>  
Detecting the Hybridization Gap
- Ba(Fe<sub>1-x</sub>Co<sub>x</sub>)<sub>2</sub>As<sub>2</sub> and Fe<sub>1+y</sub>Te  
Detecting orbital ordering?

# Quasiparticle Scattering Spectroscopy (Point Contact Spectroscopy “PCS”)



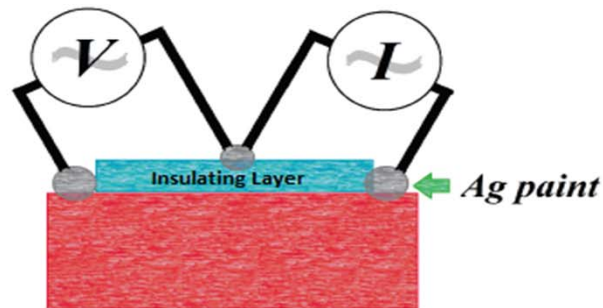
*Point-Contact Spectroscopy, Naidyuk & Yanson (2005)*

- If two bulk metals are in contact with each other and the contact size is smaller than electronic mean free paths, quasiparticle energy gain/loss mostly occurs at the constriction.
- Nonlinearities in current-voltage characteristics reflect energy-dependent quasiparticle scatterings in the contact region.

# Quasiparticle Scattering Spectroscopy (Point Contact Spectroscopy “PCS”)

- Transparent Contact between two materials (***not tunneling***).
- ***Contact area less than elastic mean free path.***
- Measure  $dI/dV$  vs.  $V$  bias.

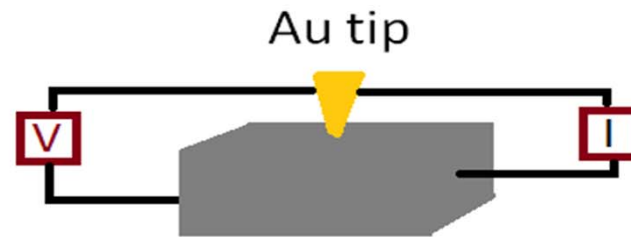
## Soft PCS



Microshorts through insulating layer

- ✓ Thermally stable
- X Little control over junction resistance

## Needle-anvil PCS



Electrochemically etched nanoscale gold

- ✓ Tunable junction resistance (piezoelectric bimorphs / screw)
- X Thermally less stable

# Quasiparticle scattering (PCS): What we detect

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## 1. Superconductivity (intro):

Gap, order parameter symmetry, density of state, ... this is well understood in the framework of BTK and Andreev reflection.

## 2. Kondo Impurity / Kondo Lattice effects (intro):

Fano lineshape consistent with the growth of the Kondo liquid (starts at  $T^*$ , and grows until  $T_c$ ): microscopic explanation?

## 3. Antiferromagnetic ordering (intro):

Conductance enhancement at  $T_N$  in some AF systems (not all)

## 4. The hybridization gap & Fano resonance in a heavy fermions

## 5. Orbital ordering?

**This talk:** Enhancement at high-T in Co:BaFe<sub>2</sub>As<sub>2</sub> and FeTe.



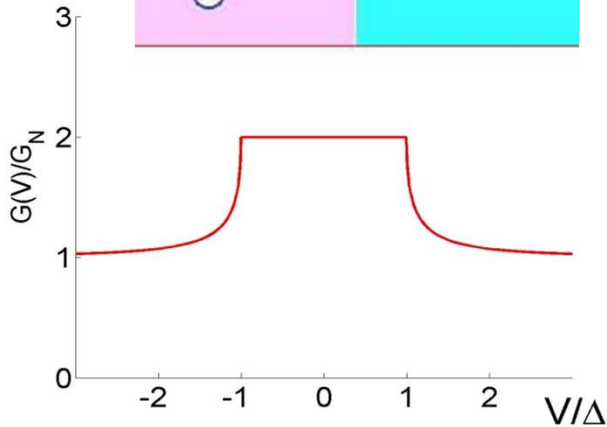
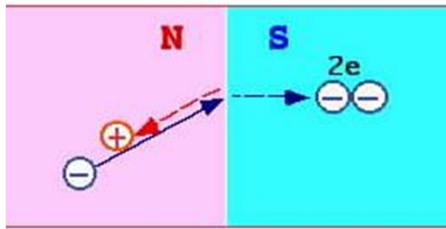
# Superconductivity: PCS to Tunneling - BTK model

Three fitting parameters

$\Delta$  = superconducting gap

$\Gamma$  = Dynes broadening factor (qp scattering rate)

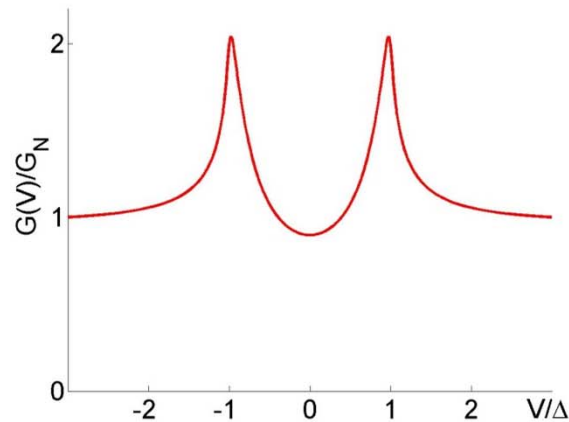
$Z_{\text{eff}}$  = barrier strength at the N/S interface



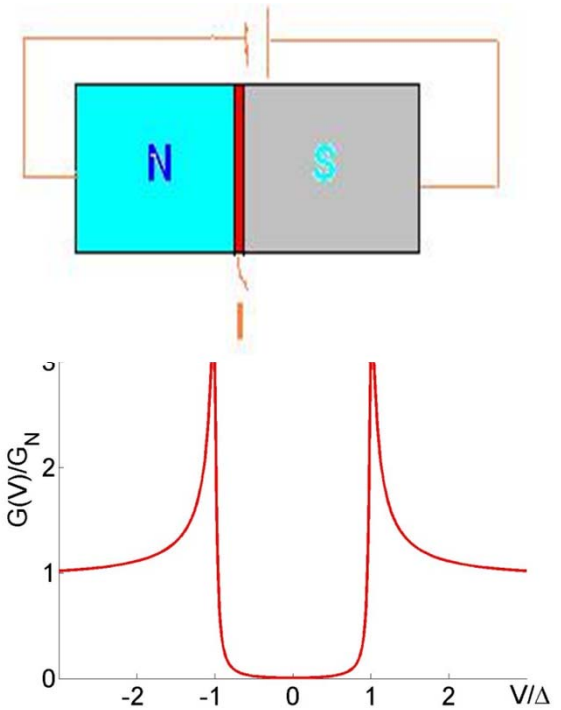
$Z = 0$

Andreev Reflection

Assuming  $\Gamma = 0$  and  $\Delta = 1$



$Z = 0.5$

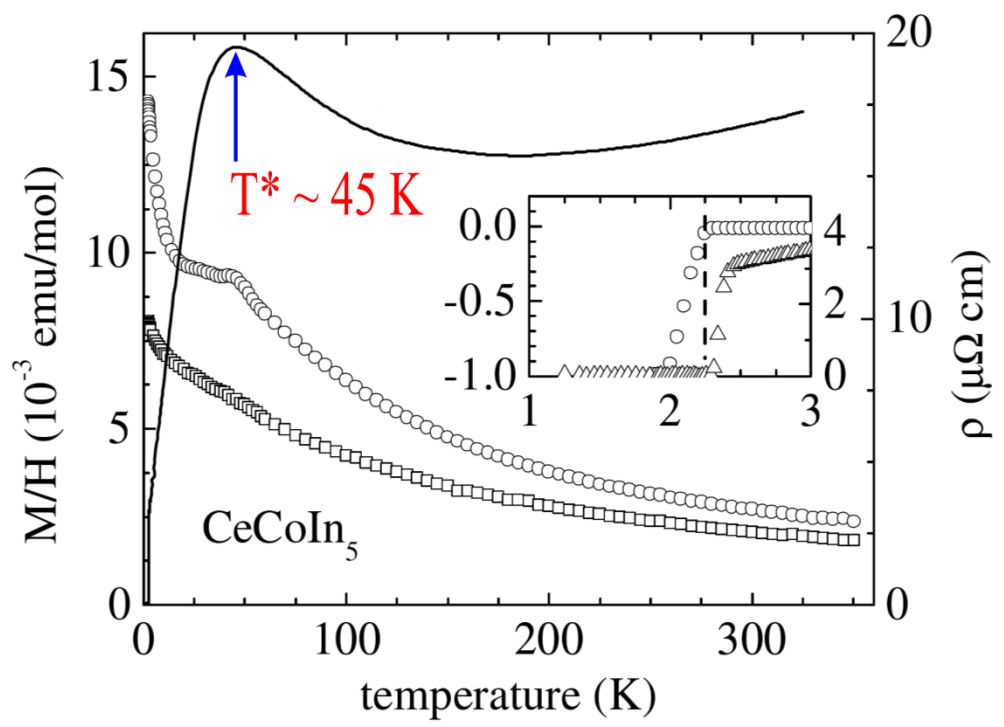
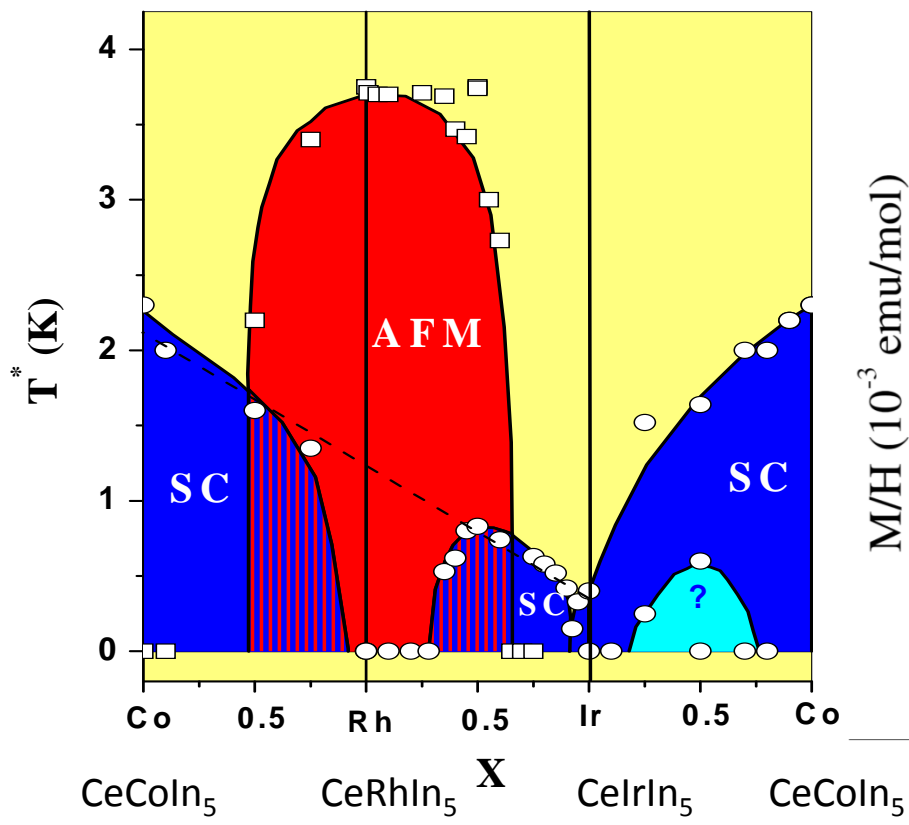


$Z = 5.0$

Tunneling

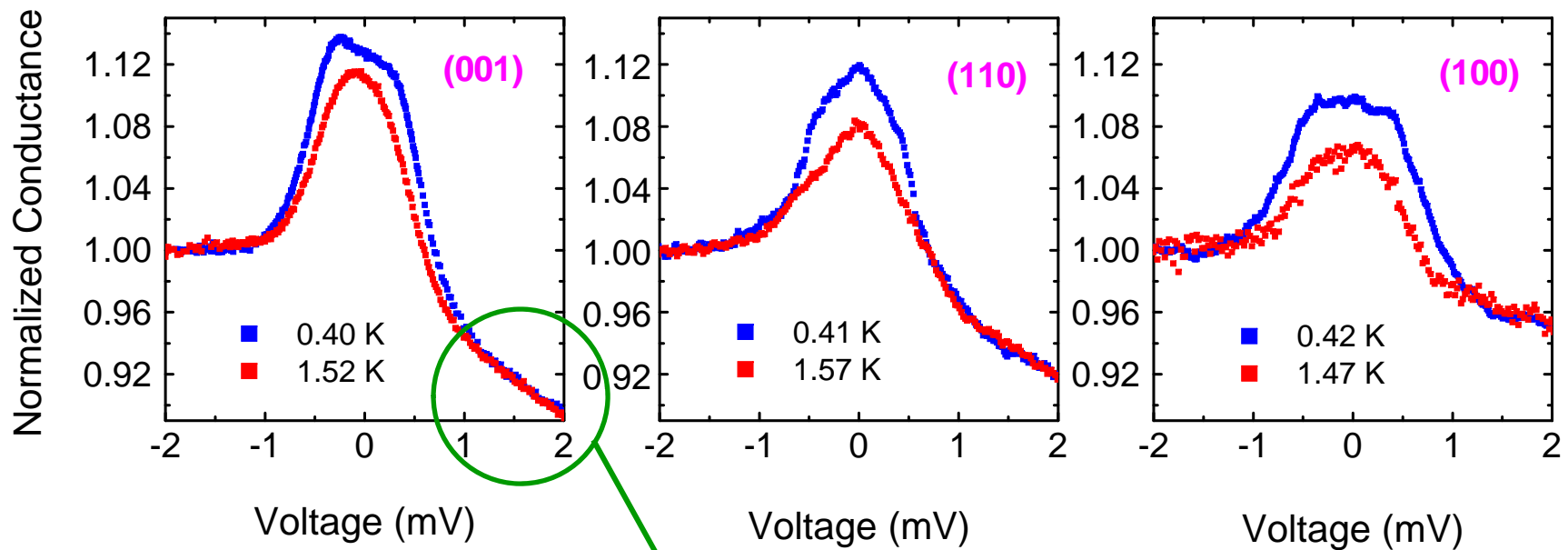
# The Heavy Fermion Superconductor CeCoIn<sub>5</sub>: Phase diagram of series Ce M In<sub>5</sub> (M = Co, Rh, Ir) & transport

- $T_c = 2.3$  K (high for many HFS)
- Superconductivity in clean limit ( $mfp = 810\text{\AA} \gg \xi_0$ )



# Superconductivity: Gap and OP Symmetry

## Data: Consistency Along Three Orientations

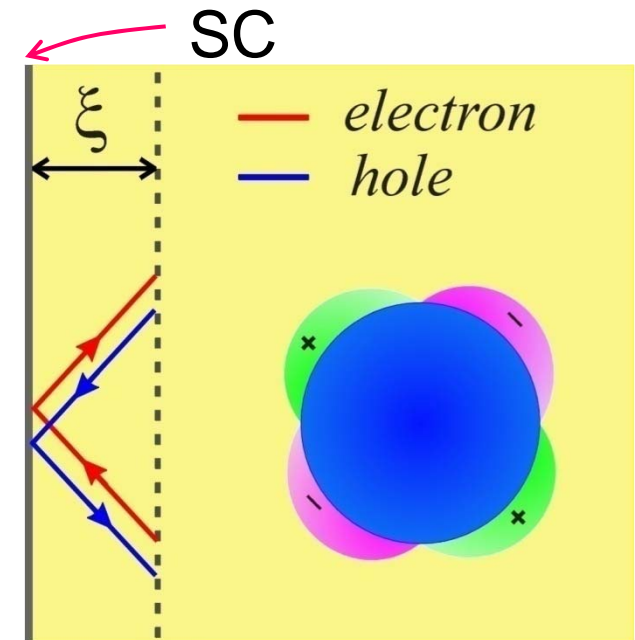
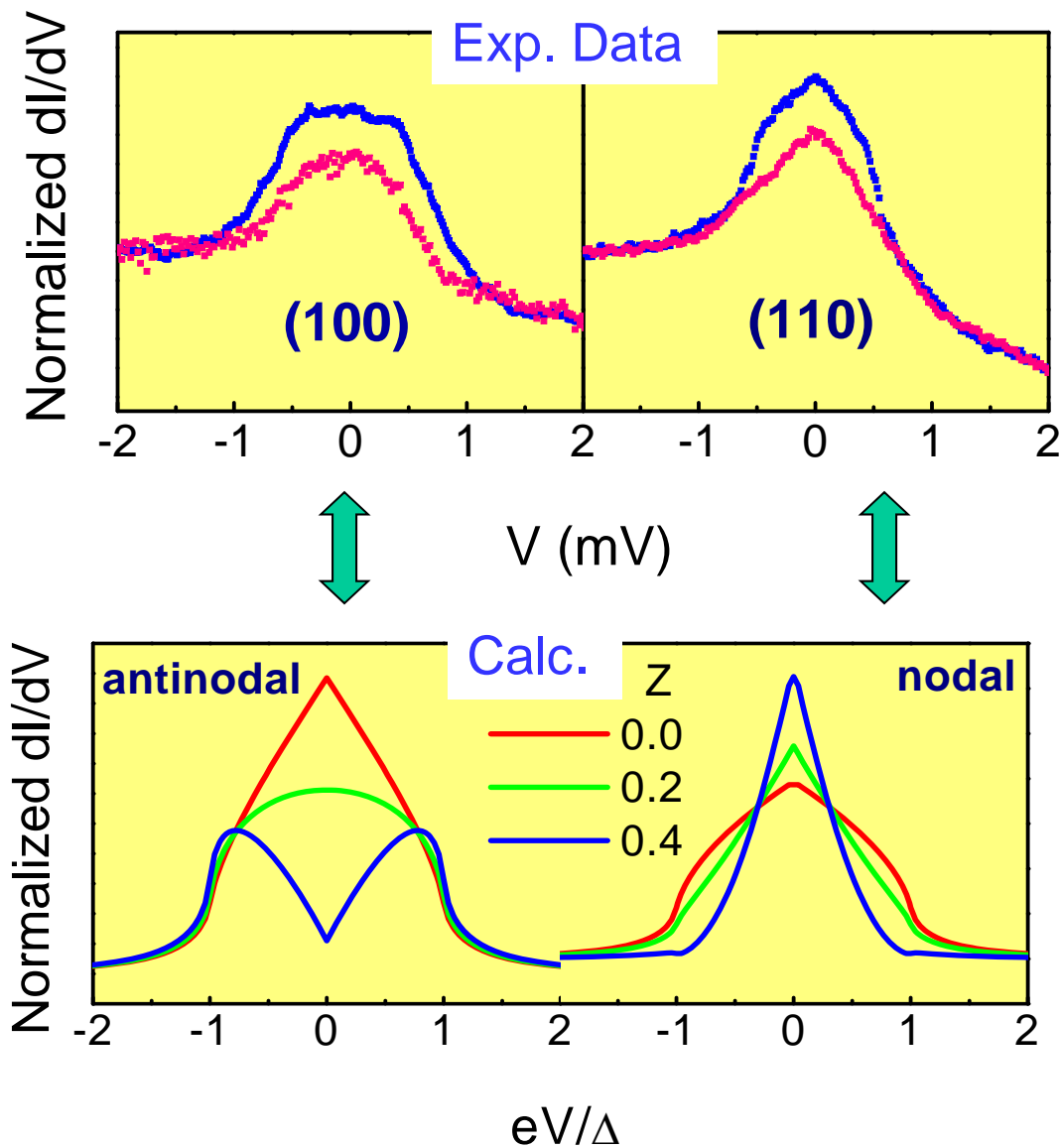


(+) CeCoIn<sub>5</sub>; (-) Au

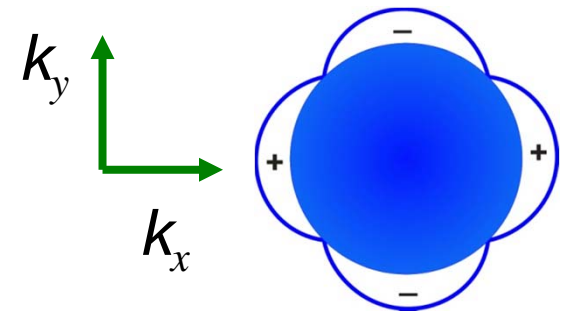
=> Adding electrons to CeCoIn<sub>5</sub> above the Fermi energy is more difficult than removing them

Note the shapes of the conductance curves

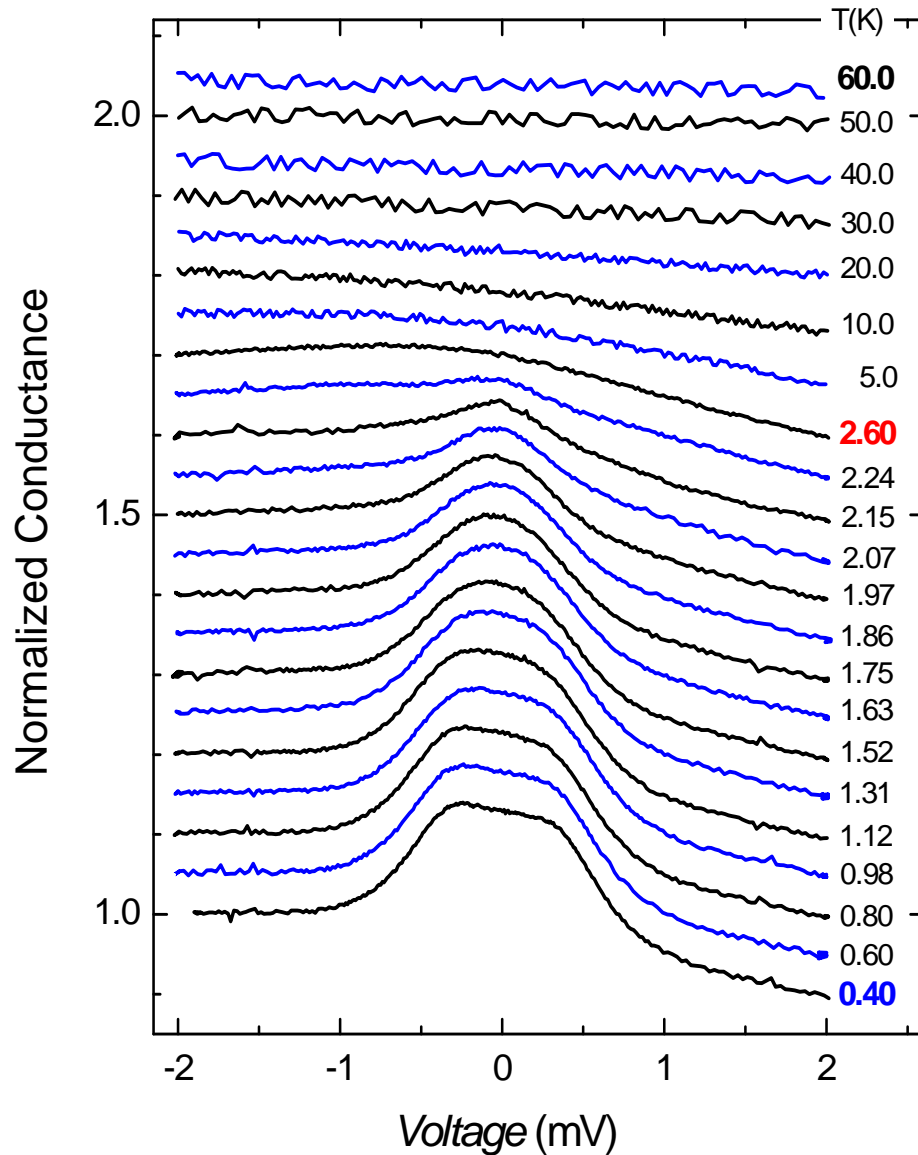
# Spectroscopic Evidence for $d_{x^2-y^2}$ Symmetry



Andreev Bound States (ABS)

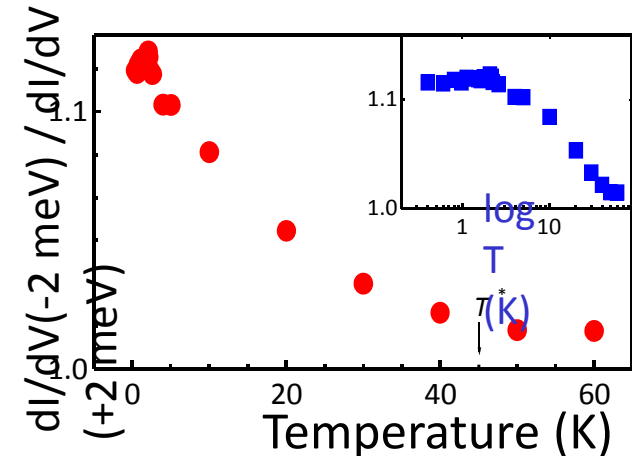


# Kondo: Background Conductance Asymmetry of CeCoIn<sub>5</sub>



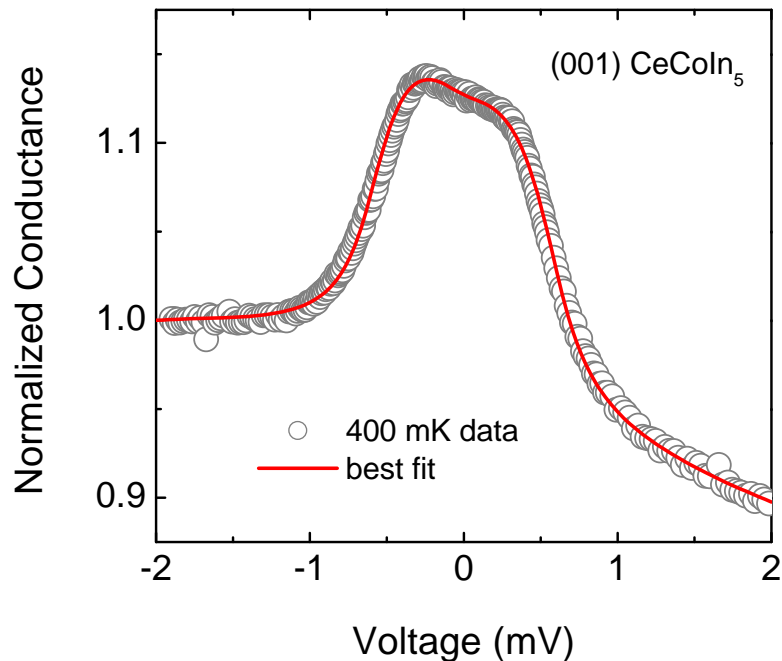
$T^*$  Background develops an **asymmetry\*** at the heavy-fermion liquid coherence temperature,  $T^* \sim 45$  K.

$T_c$  This asymmetry gradually increases with decreasing temperature until the onset of superconducting coherence,  $T_c = 2.3$  K.

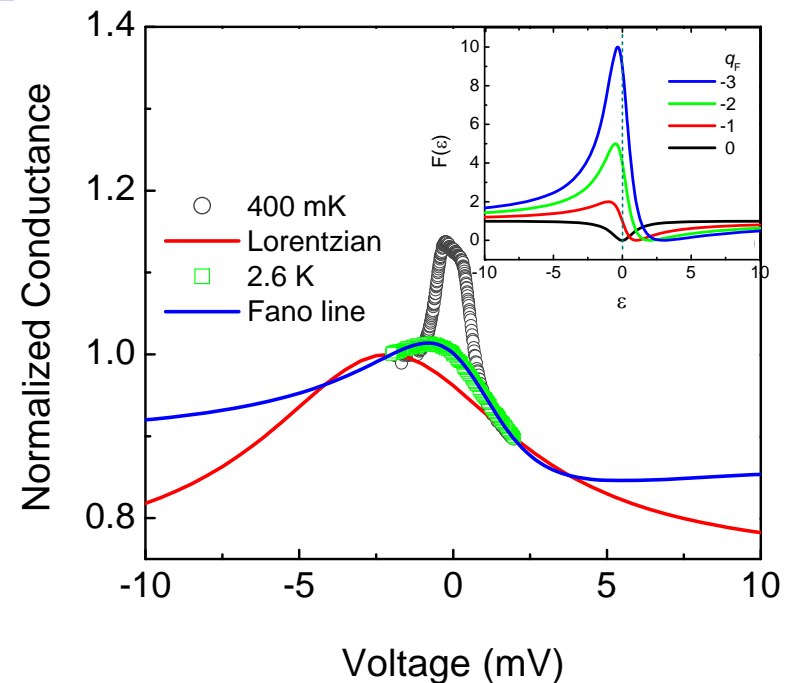


# Model fits magnitude of AR, asymmetry and T-dep !

Data (circles) and fit (red line) is excellent



Best fit over wide T-range with a **Fano lineshape**

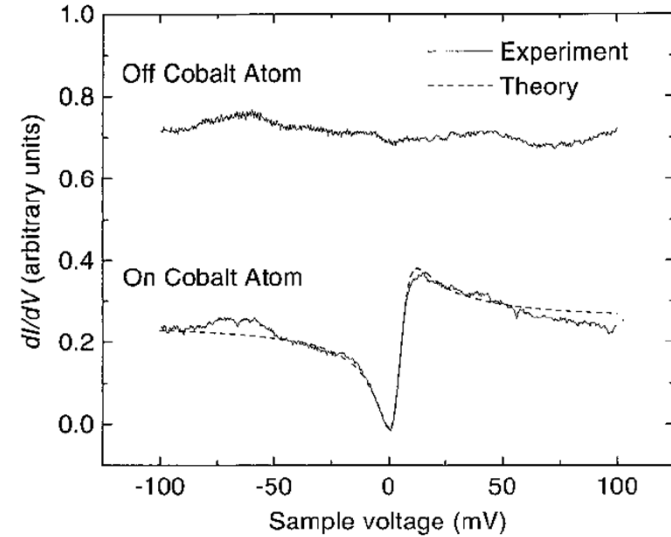
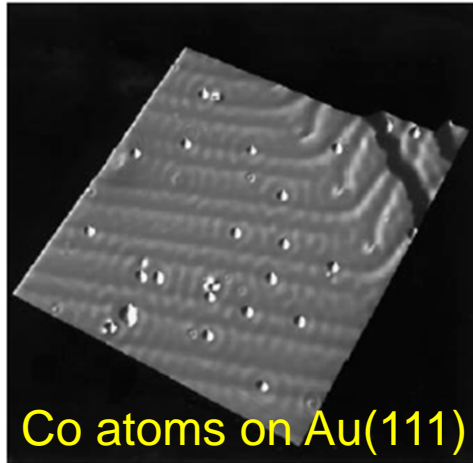


Fano may be explained by interference between f-electrons and conduction electrons via spin-flip (Kondo) scattering.

W. K. Park et al., PRL 08 and Y.-F. Yang et al., PRL 08

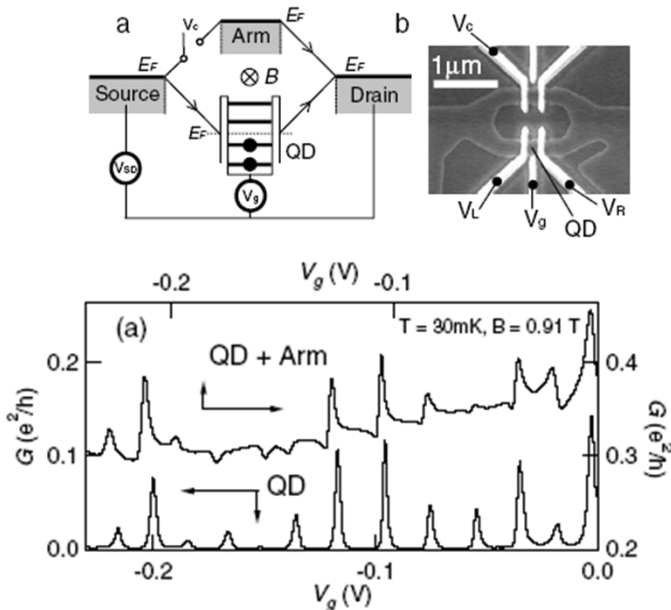
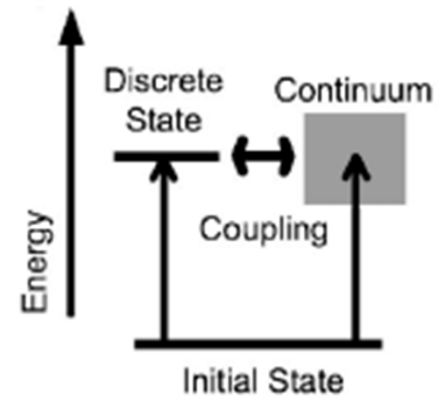
# Fano Resonance in Single Impurity and Quantum Dot

V. Madhavan et al.,  
 Science 280, 567  
 (1998)

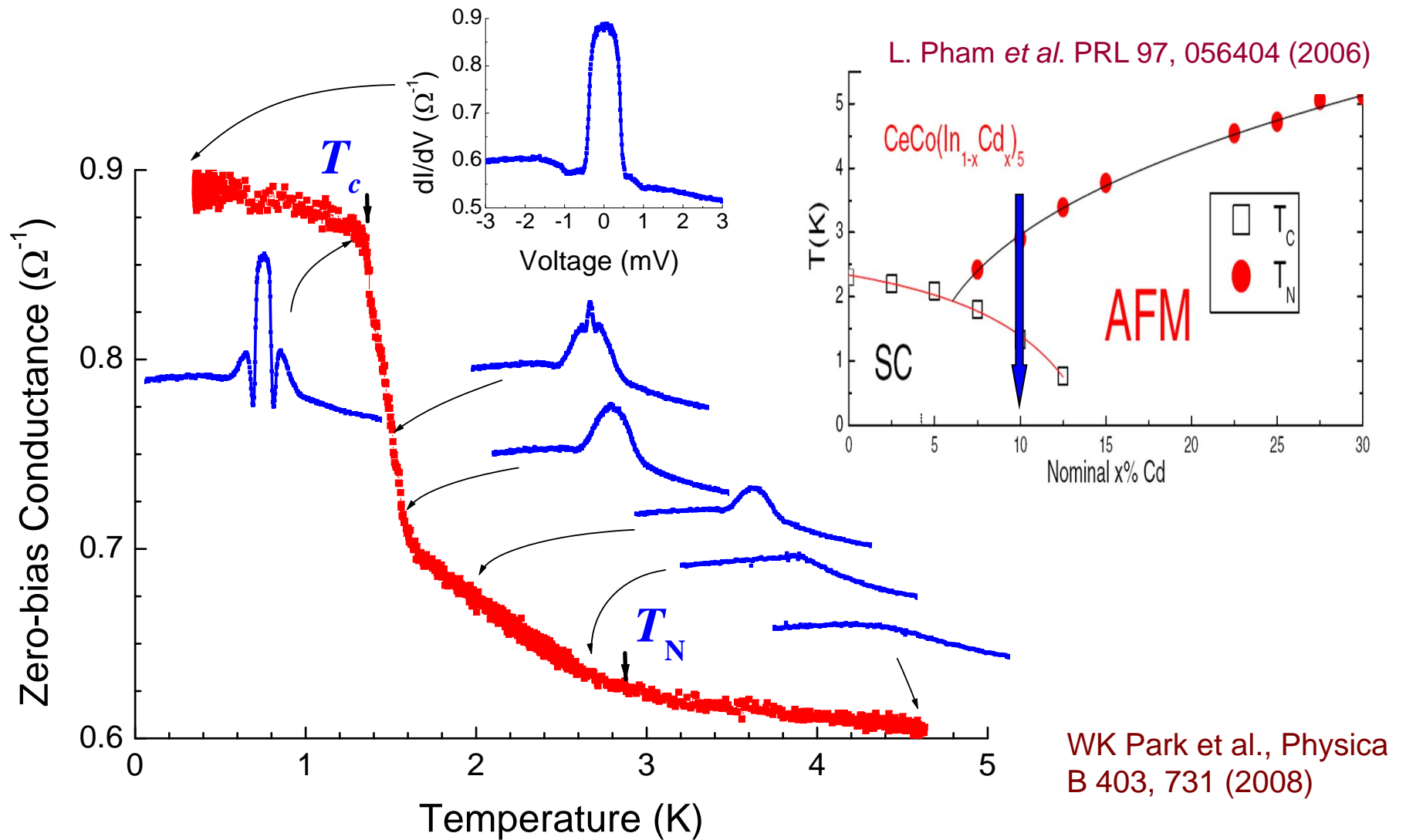


K. Kobayashi et al., PRL 88, 256806 (2002)

“The Fano effect is essentially a single-impurity problem describing how a **localized** state embedded in the continuum acquires **itinerancy** over the system.”



# Antiferromagnetism: Cd:CeCoIn<sub>5</sub>: Anomalous Conductance



non-monotonic; enhancement below  $T_N$ , competition below  $T_{c0}$



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## 3. Antiferromagnetic ordering (intro):

Conductance enhancement at  $T_N$  in some AF systems (not all

## **NOW:**

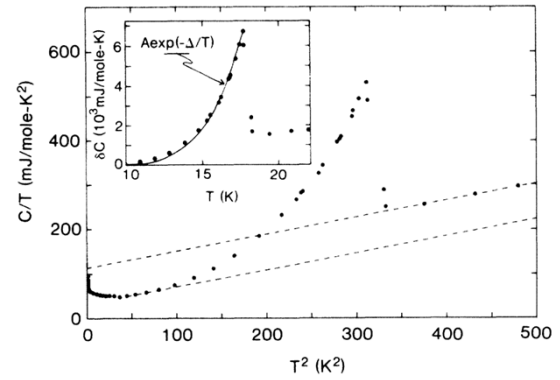
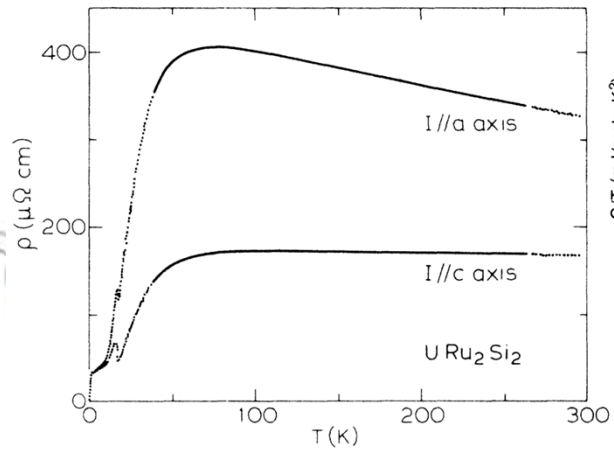
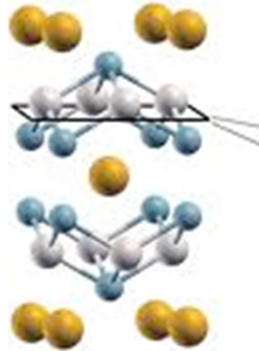
### 1. The hybridization gap & Fano resonance in a heavy

**fermion This talk:** Helps explain #2.

### 2. Orbital ordering?

**This talk:** Enhancement at high-T in Co:BaFe<sub>2</sub>As<sub>2</sub> and FeTeSe.

# The Heavy Fermion / Kondo Lattice $\text{URu}_2\text{Si}_2$

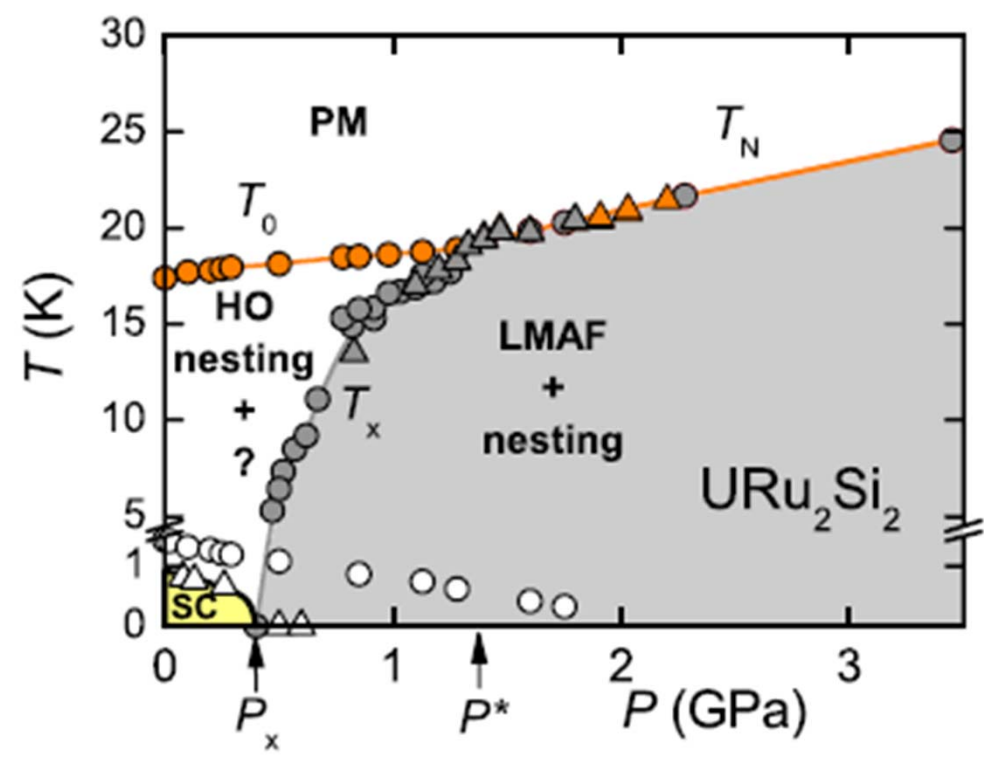


$\Delta =$   
115 K  
(9.9 meV)

Pastra et al., PRL (86); PRB (87)

## A Phase Diagram

Hassinger et al., PRB 77, 115117 (2008)



# Hybridization Picture of a Kondo Lattice

Periodic Anderson model

e.g., Newns & Read, Adv. Phys. (1987)

$$H_{\text{PAM}} = \sum_{k\sigma} (\varepsilon_k - \mu) c_{k\sigma}^\dagger c_{k\sigma} + \sum_{k\sigma} (\varepsilon_f - \mu) f_{k\sigma}^\dagger f_{k\sigma} + \sum_{k\sigma} V_k (f_{k\sigma}^\dagger c_{k\sigma} + c_{k\sigma}^\dagger f_{k\sigma}) + U \sum_i n_{f,i\uparrow} n_{f,i\downarrow}$$

Mean field solution

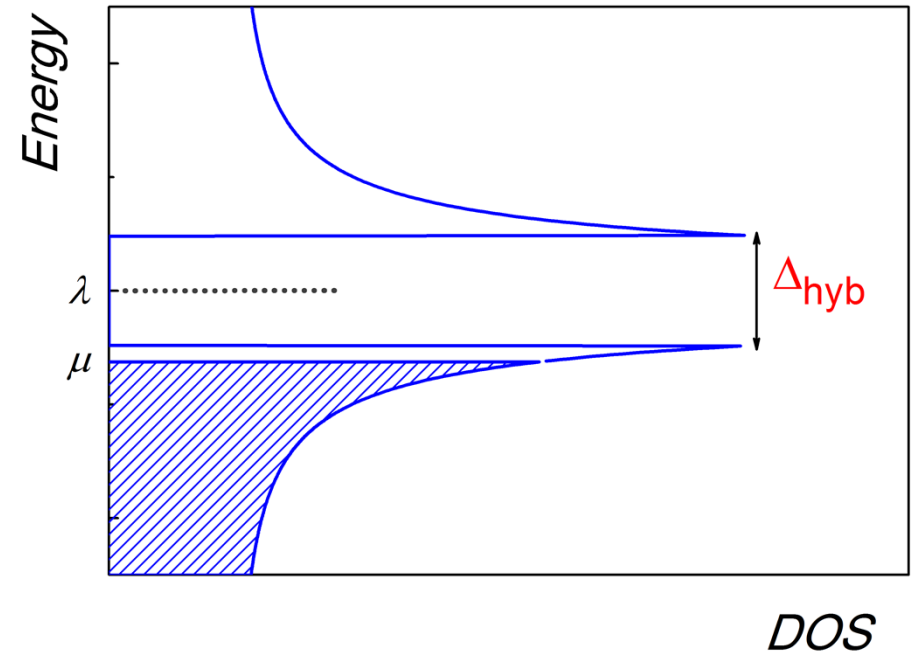
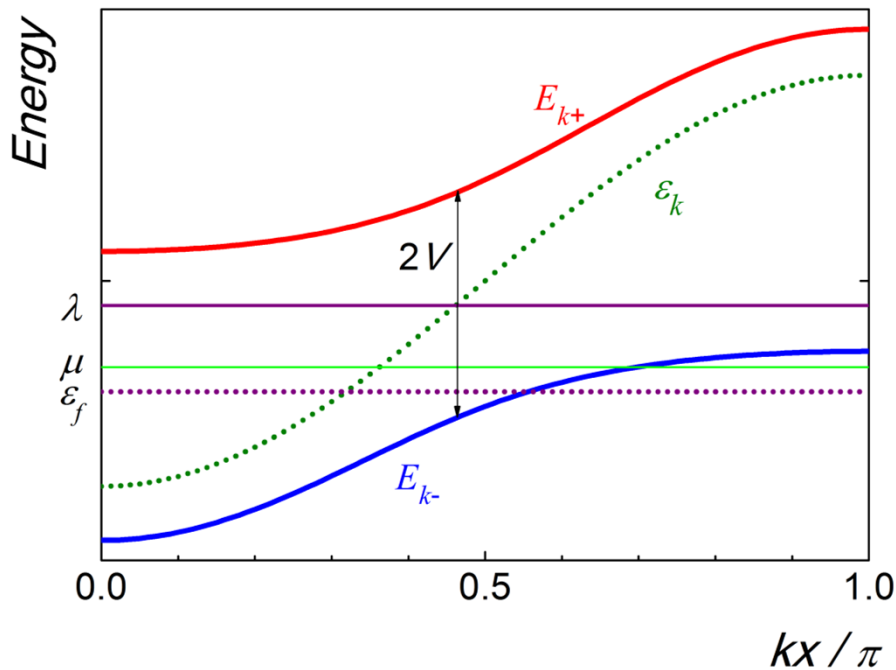
$$E_{k\pm} = \frac{1}{2} \left\{ \varepsilon_k + \lambda \pm \sqrt{(\varepsilon_k - \lambda)^2 + 4V^2} \right\}, \quad V = z^{1/2} V_0$$

$\mu$ : chemical potential

$\lambda$ : renormalized  $f$ -level

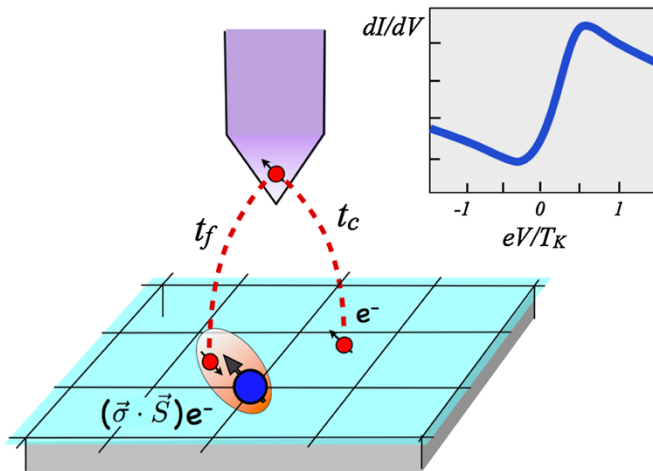
$V$ : renormalized hybridization amplitude

$z = 1 - n_f$  ( $n_f$ : occupancy)

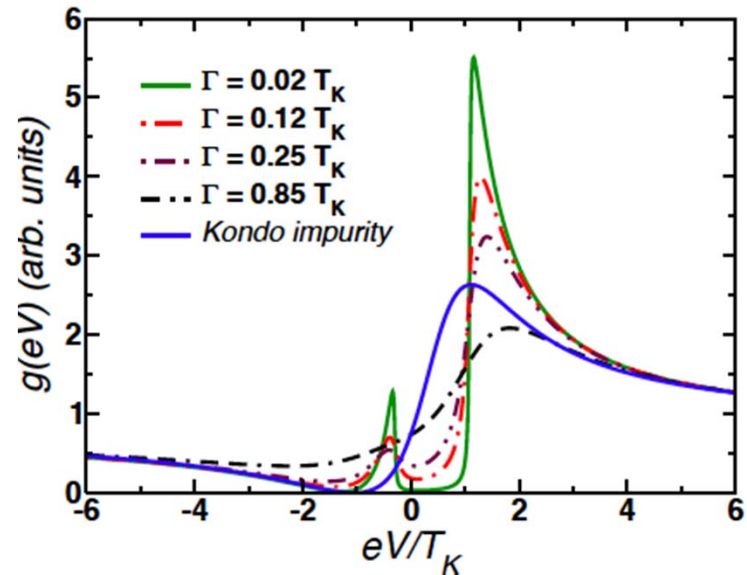


# Electron co-tunneling in a Kondo Lattice

Provides a model to account for transport / tunneling – taking itinerant and re-normalized f-electron band



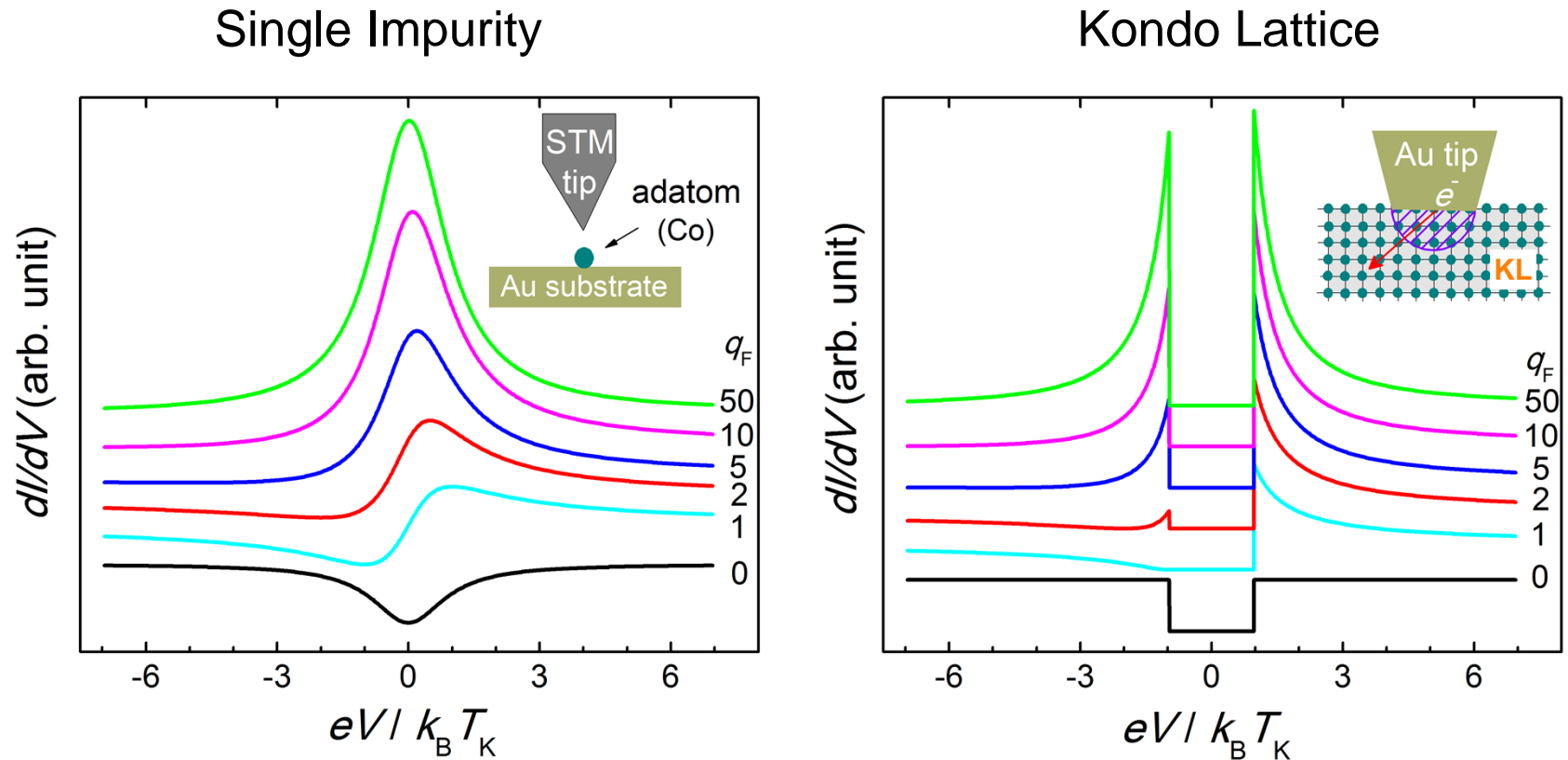
Single-impurity:  
Fano ineshape



Kondo lattice hybridization gap:  
Double peak

Maltseva, Dzero, Coleman, PRL (09)

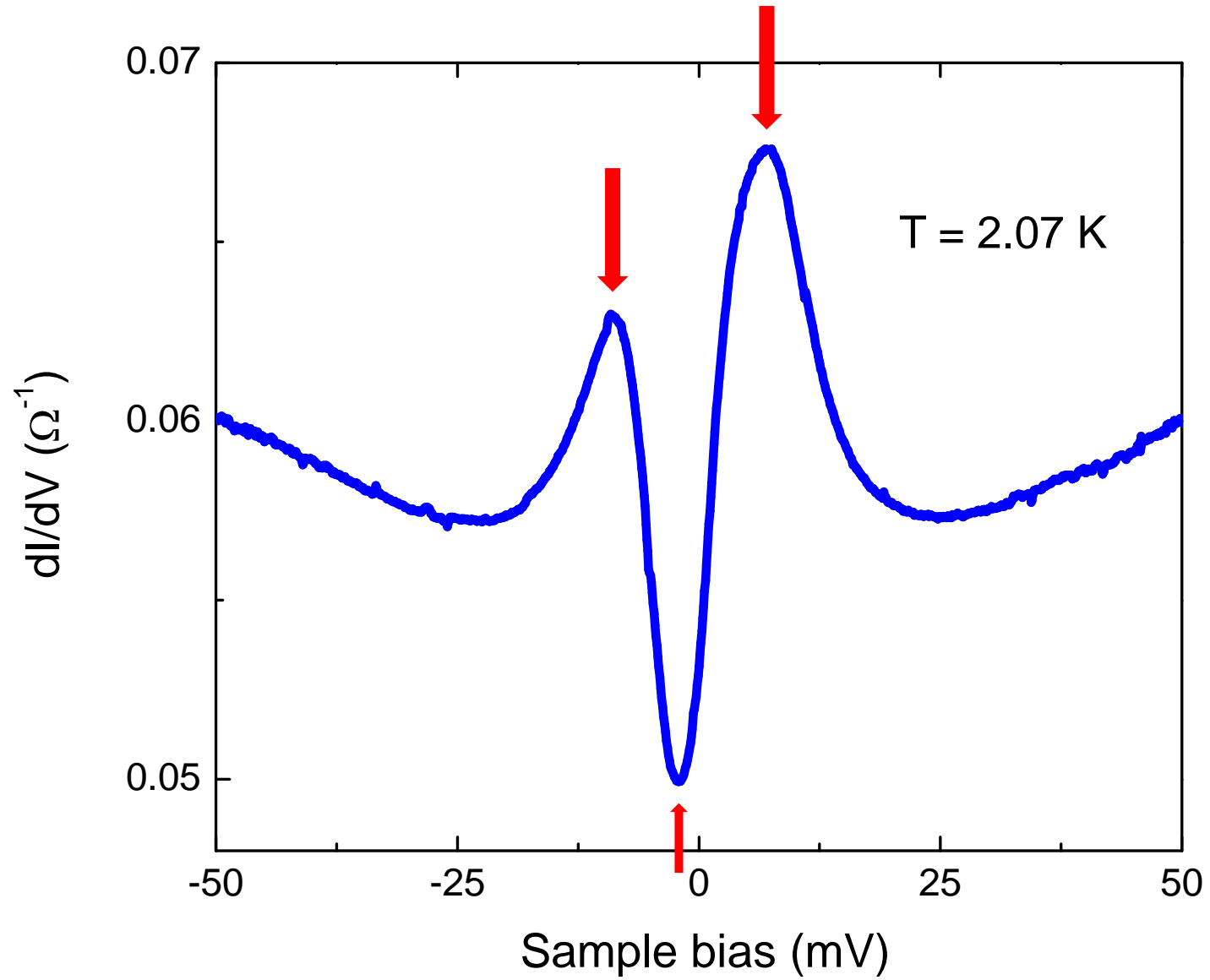
# Fano Resonance: Single Impurity vs. Kondo Lattice



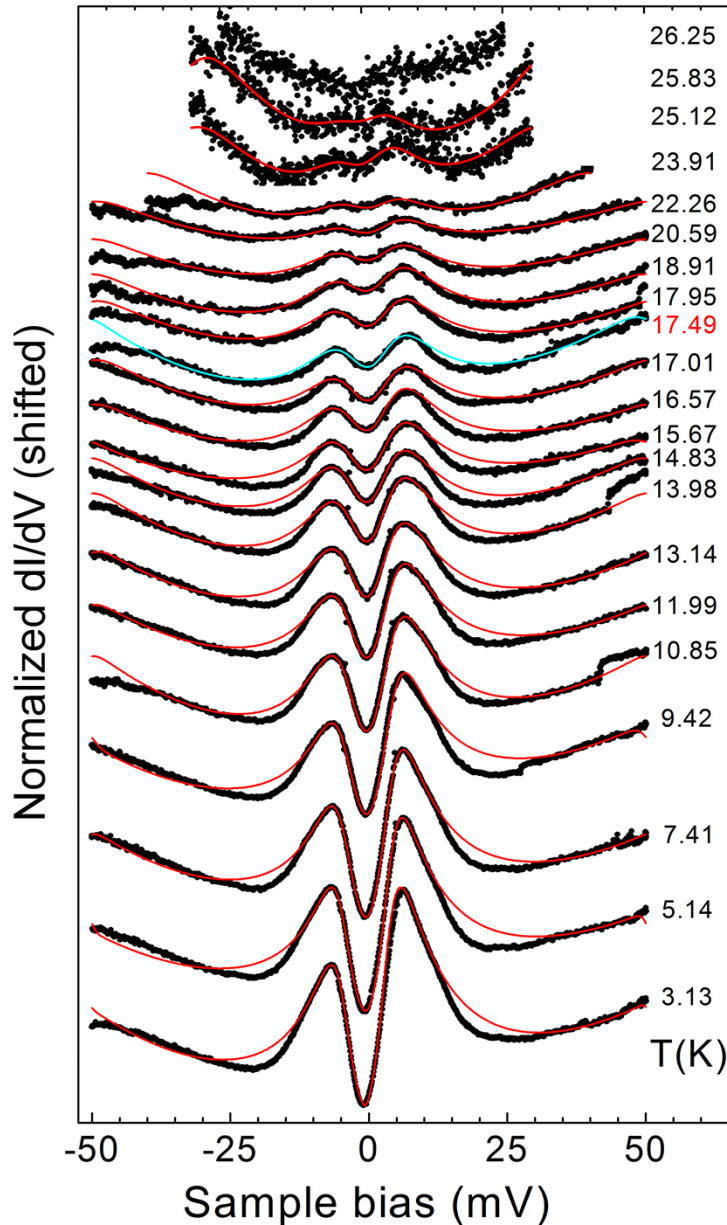
- A **distinct double-peak structure in a Kondo lattice: signature of a hybridization gap**, distinguishable from a single impurity Fano resonance.
- Asymmetry due to interference between renormalized heavy bands and conduction band.

# Typical Conductance Data

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# Temperature Dependence



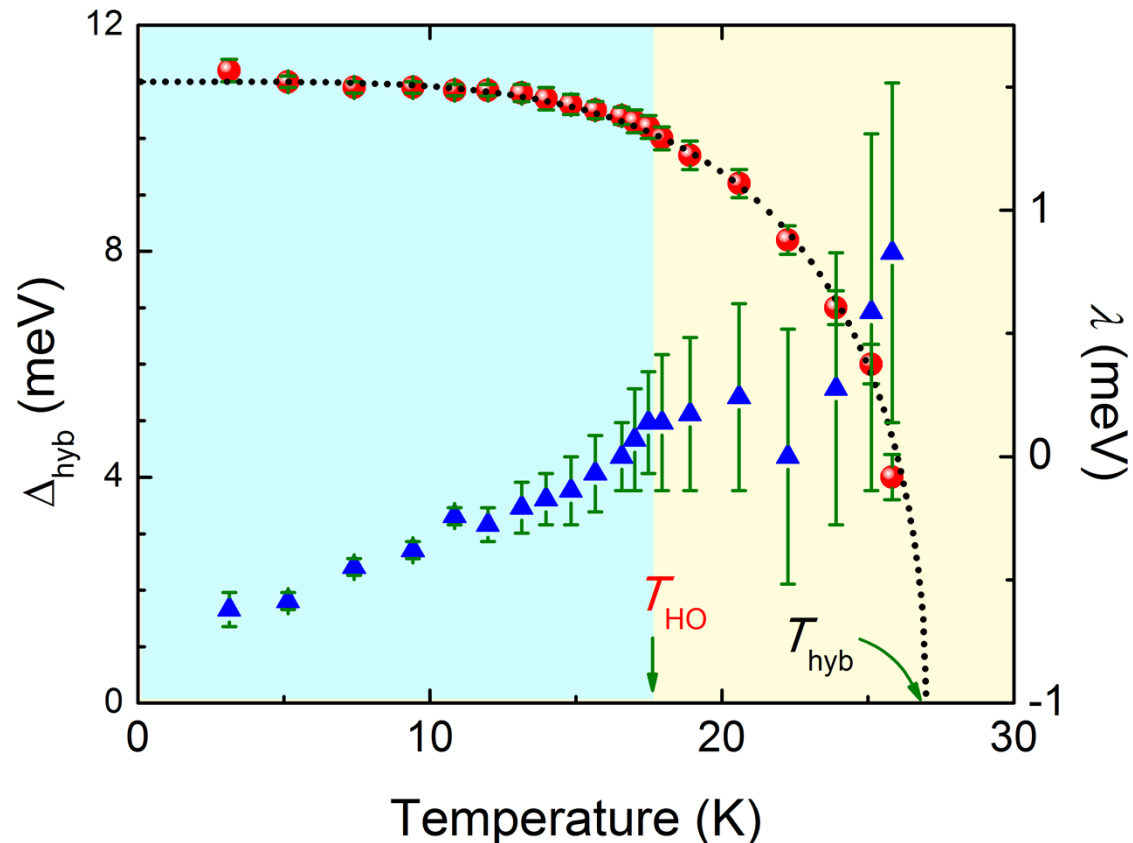
- Is this hybridization gap the long-thought hidden order parameter?

→ The answer lies in the temperature dependence.

$T_{HO}$

- Conductance spectra (filled circles) along with fitted curves (solid lines). Top three curves on a magnified vertical scale.
- The double-peak structure persists well above  $T_{HO}$ .

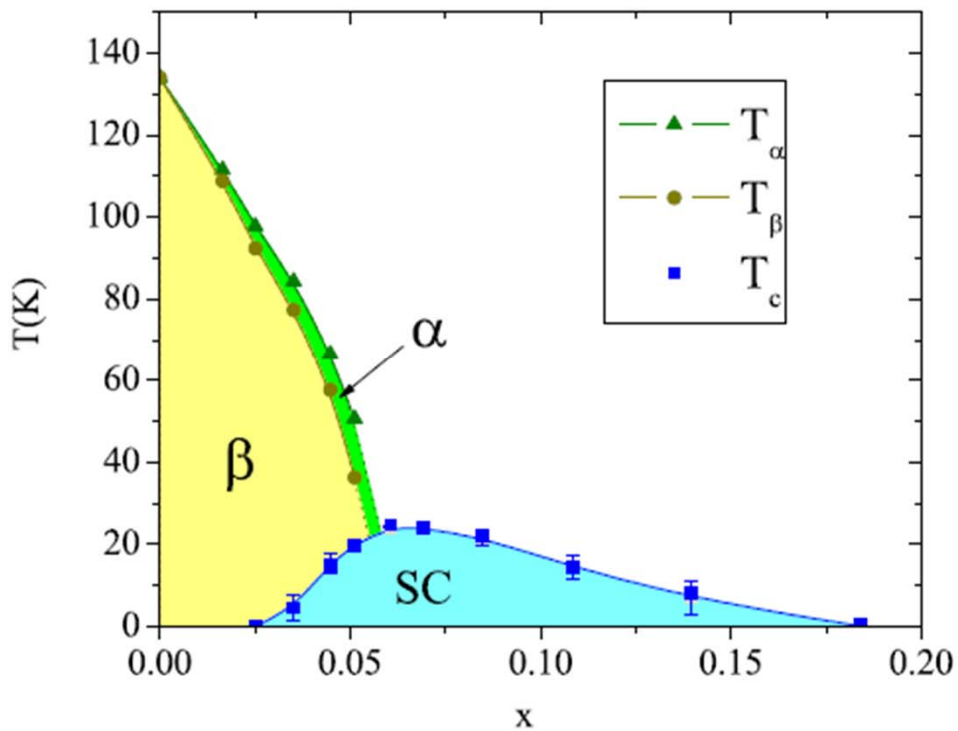
# Hybridization Gap



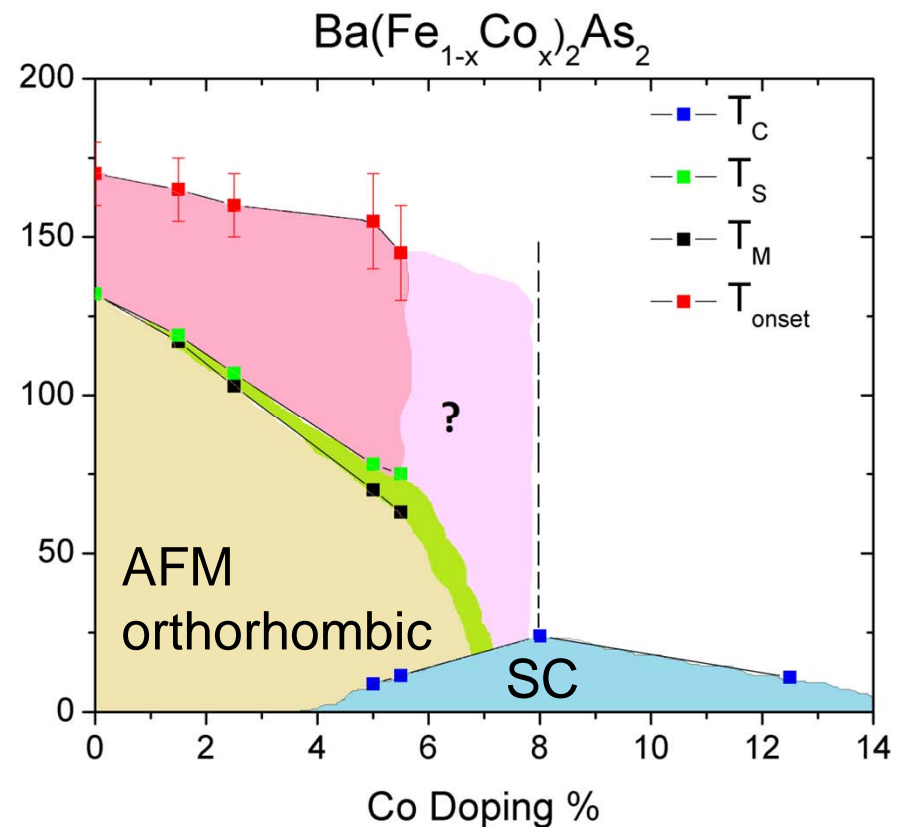
- Hybridization gap opening temperature  $T_{\text{hyb}} = 27 \text{ K} \gg T_{\text{HO}}$ .
- $\Delta_{\text{hyb}}$  is unlikely to be the hidden order parameter, as opposed to recent theoretical claims.
- Renormalized  $f$ -level shows characteristic temperature dependence. Crossing the chemical potential at  $T_{\text{HO}}$ ?



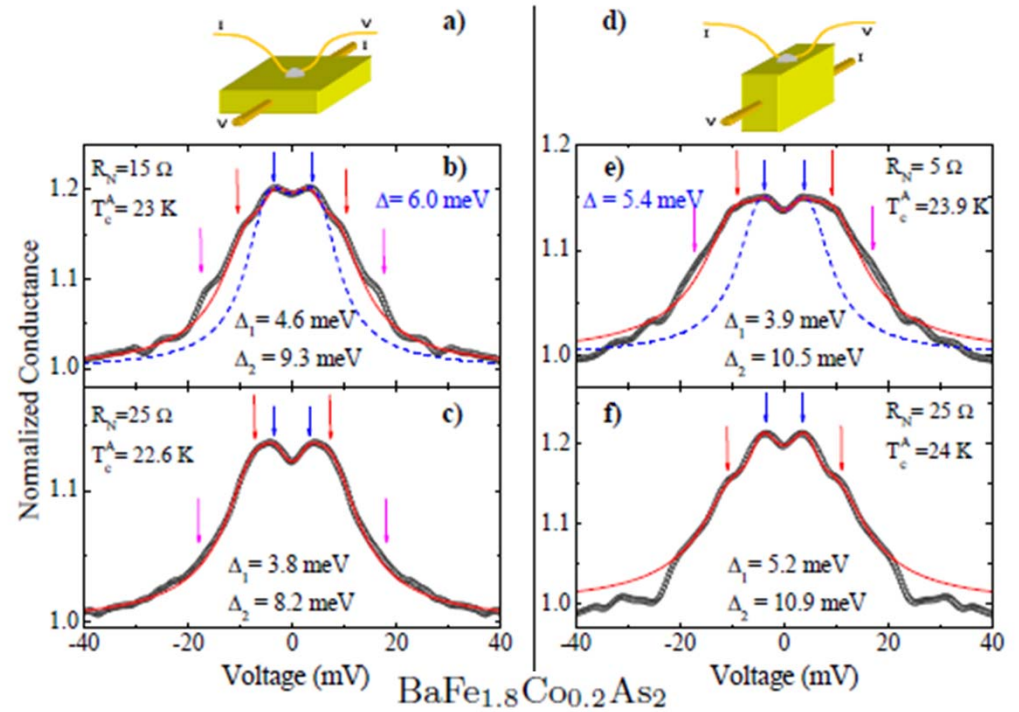
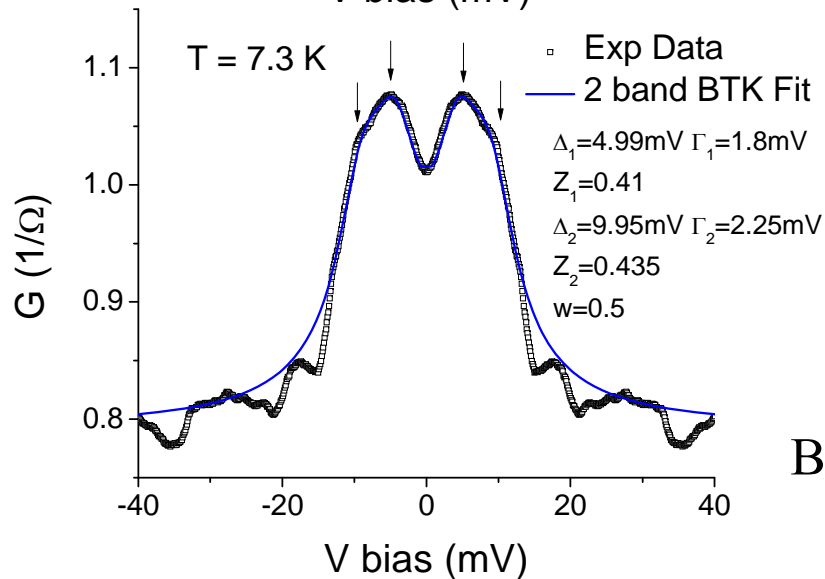
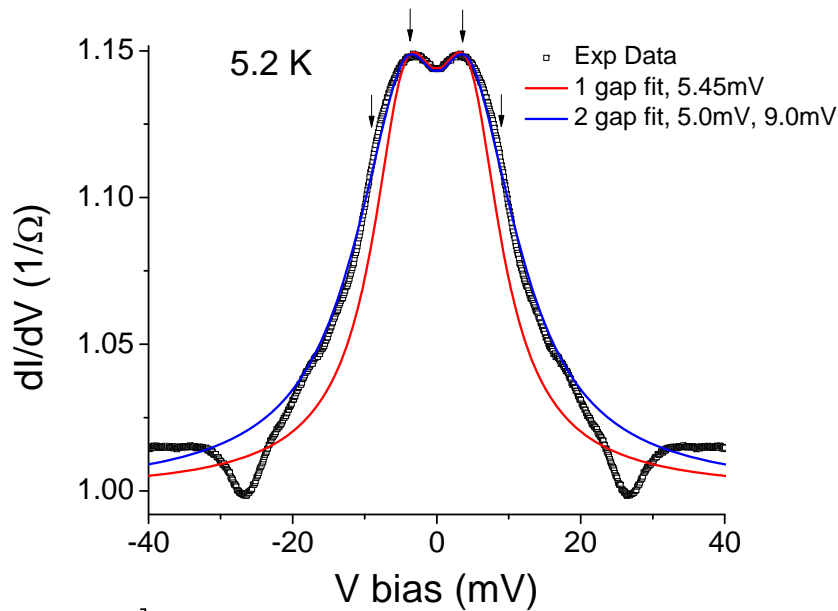
**FINALLY:** Measurement of ordering in the normal state of underdoped  $\text{Ba}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$  and  $\text{Fe}_{1+y}\text{Te}$



Chu *et al.* PRB **79**, 014506 (2009)

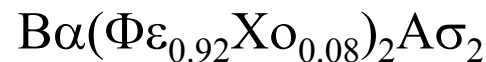


# Agreement with published data for $T < T_c$

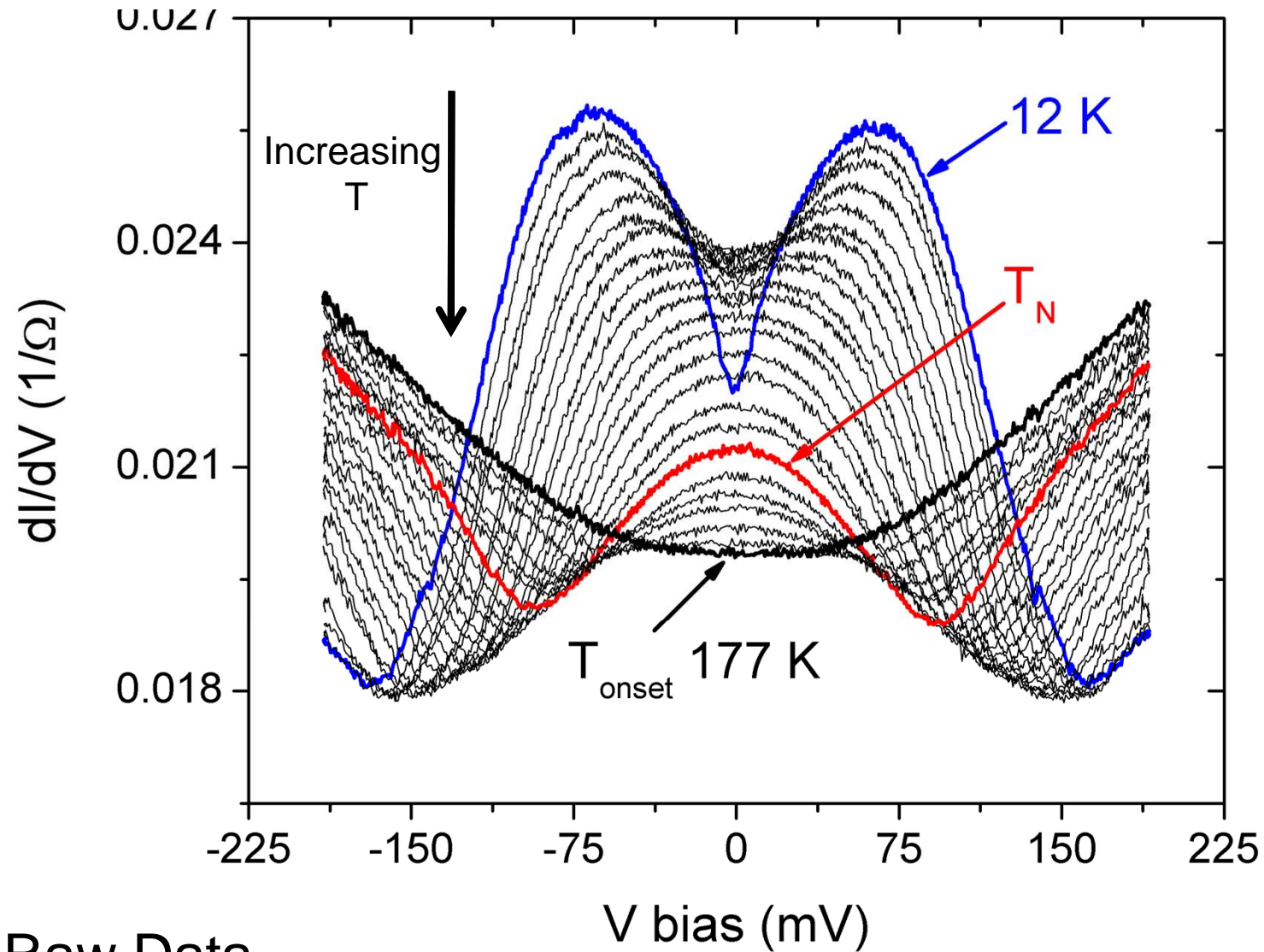


Normalized conductance curves at 4.2 K

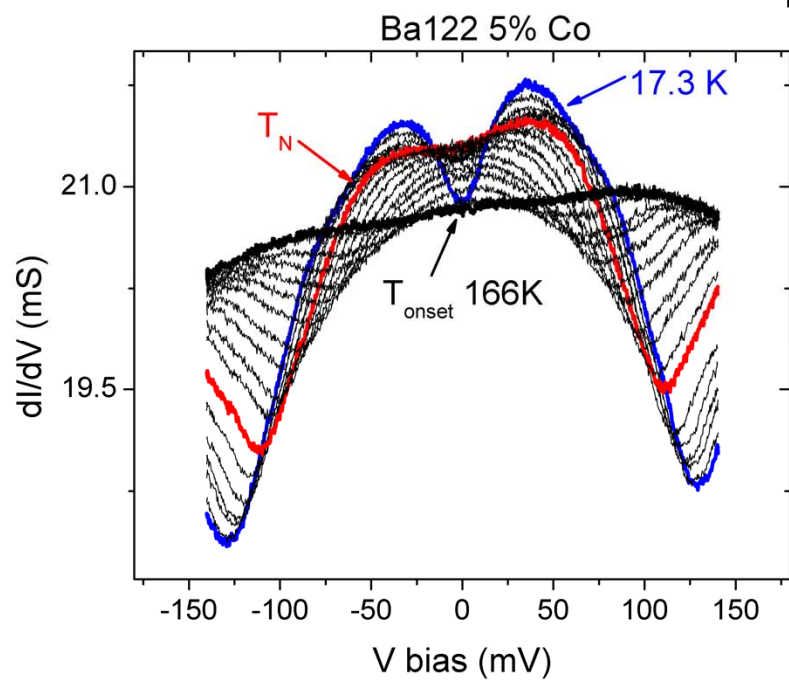
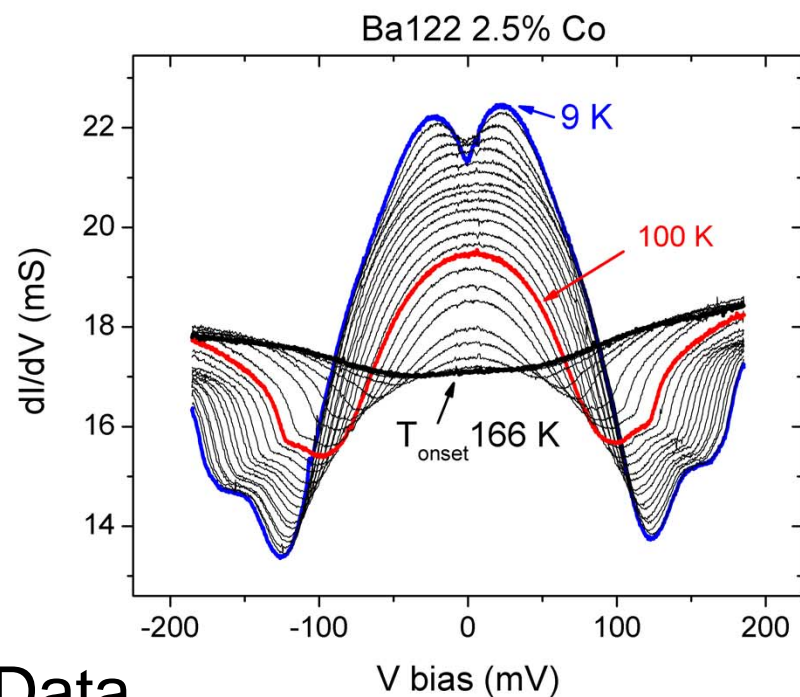
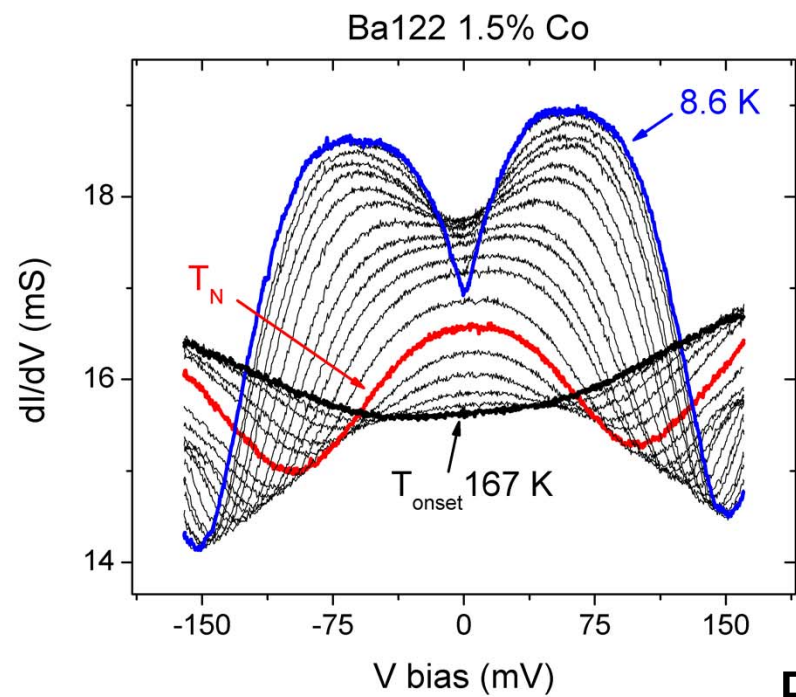
Tortello *et al.* PRL **105**, 237002 (2010)



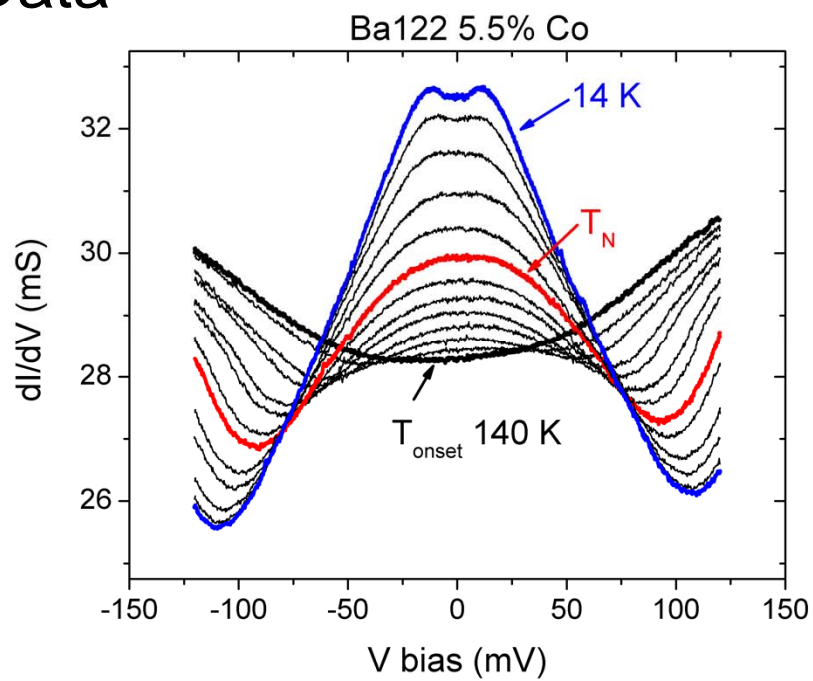
# PCS on Parent Compound: $\text{BaFe}_2\text{As}_2$



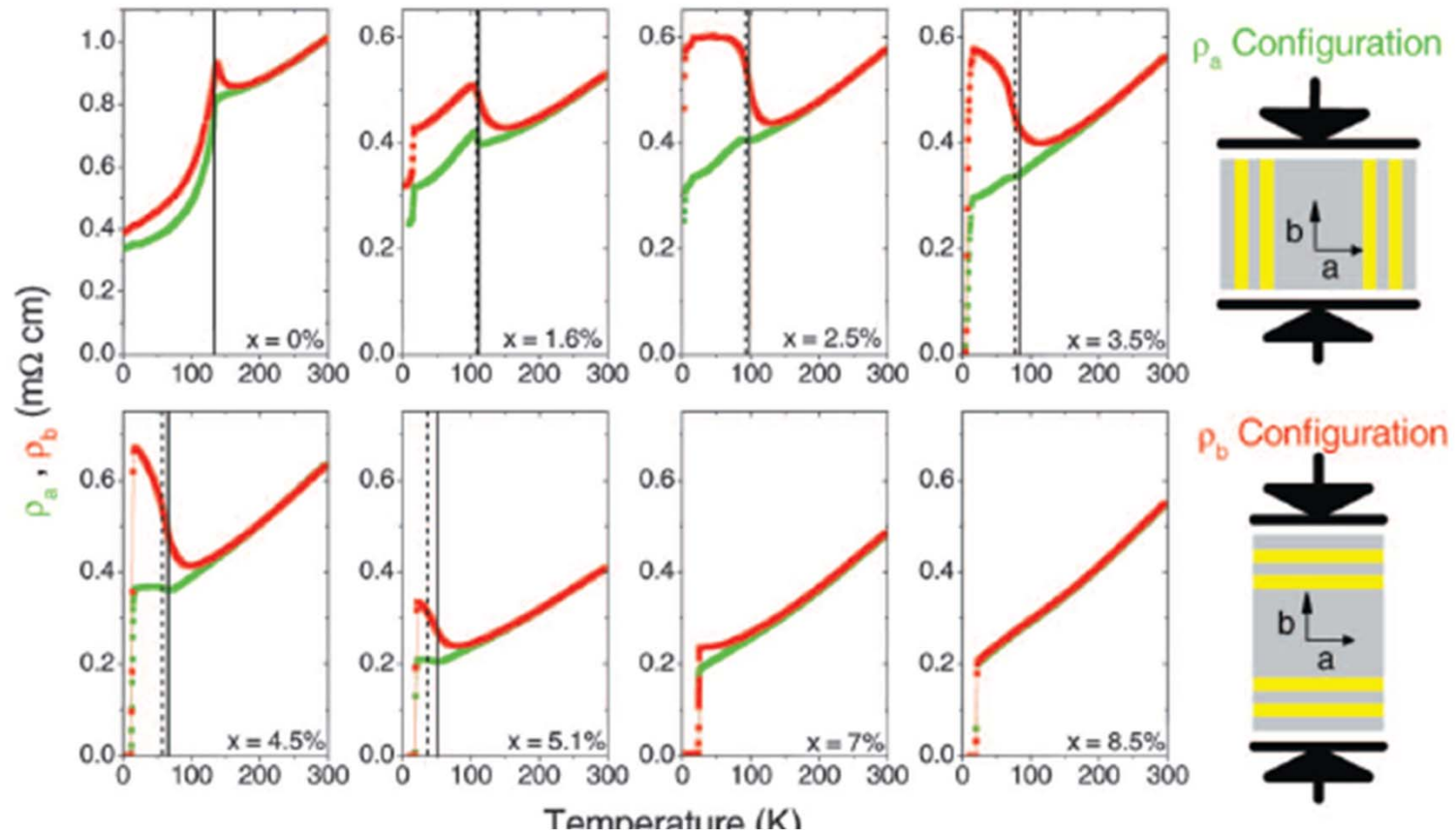
Raw Data



Raw Data

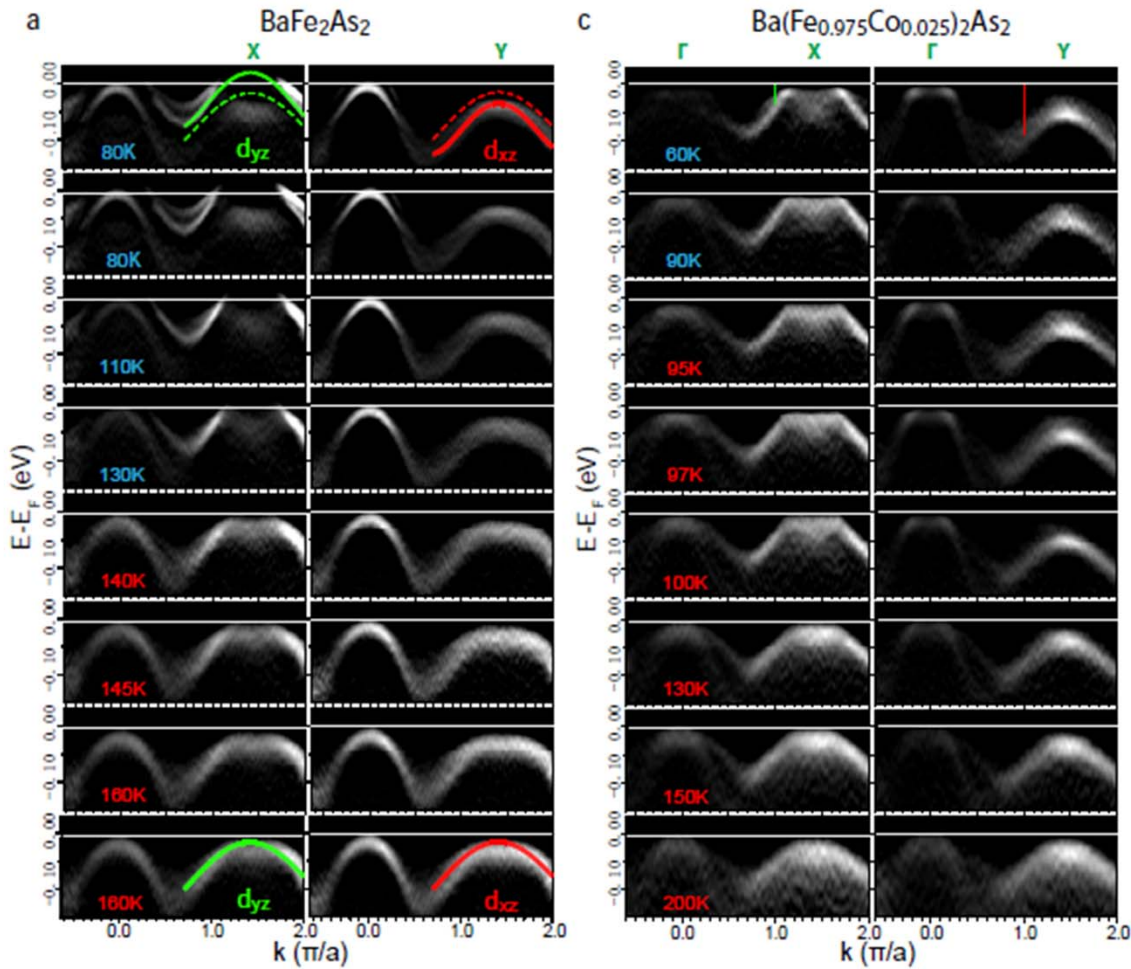


# Electronic Orthorhombicity



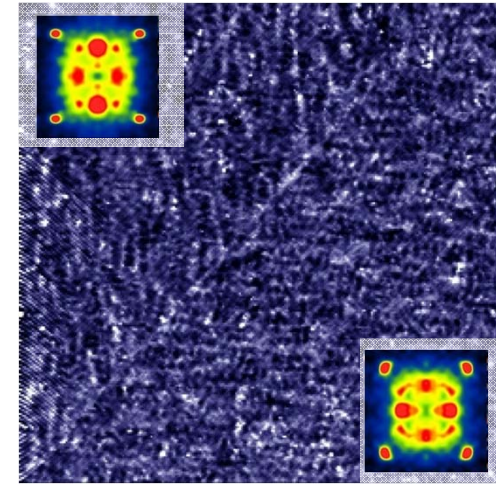
Fisher Group: Science **329**, 824 (2010).

# ARPES



Shen Group:  
arXiv:1011.0050v1

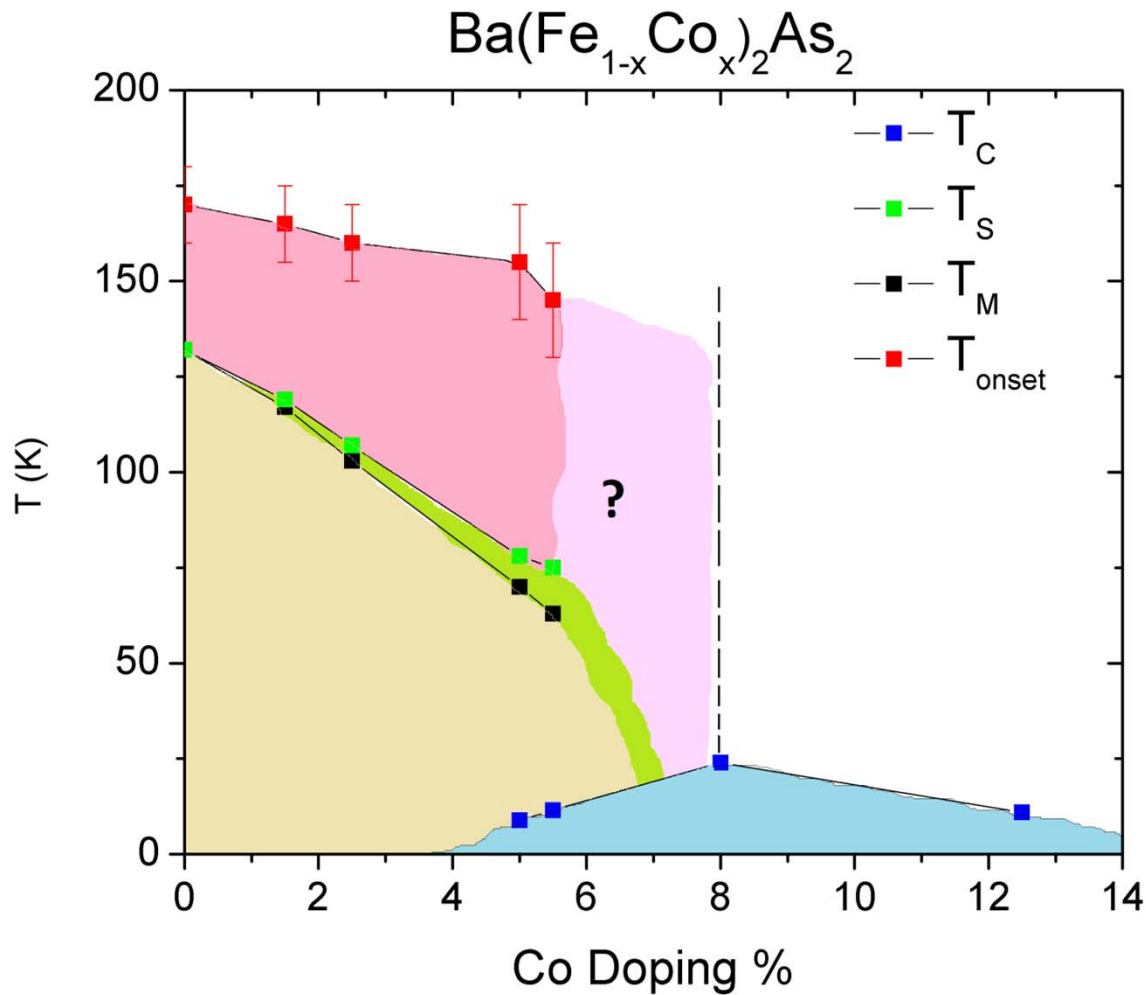
# STM



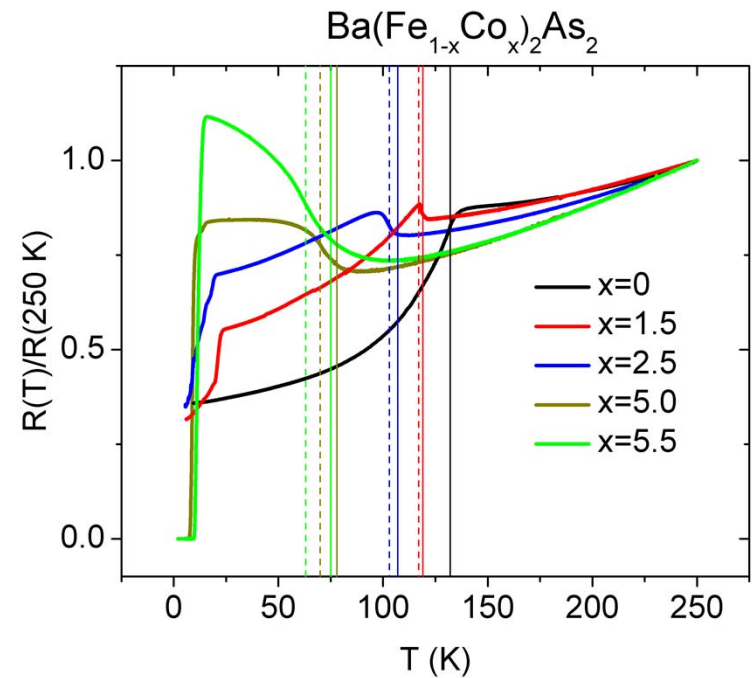
Davis Group: Science  
327, 181 (2010)

PCS  
sensitive to  
orbital  
ordering?

# New line in the Phase Diagram



$T_S, T_M$  determined from peaks in  $-dR/dT$



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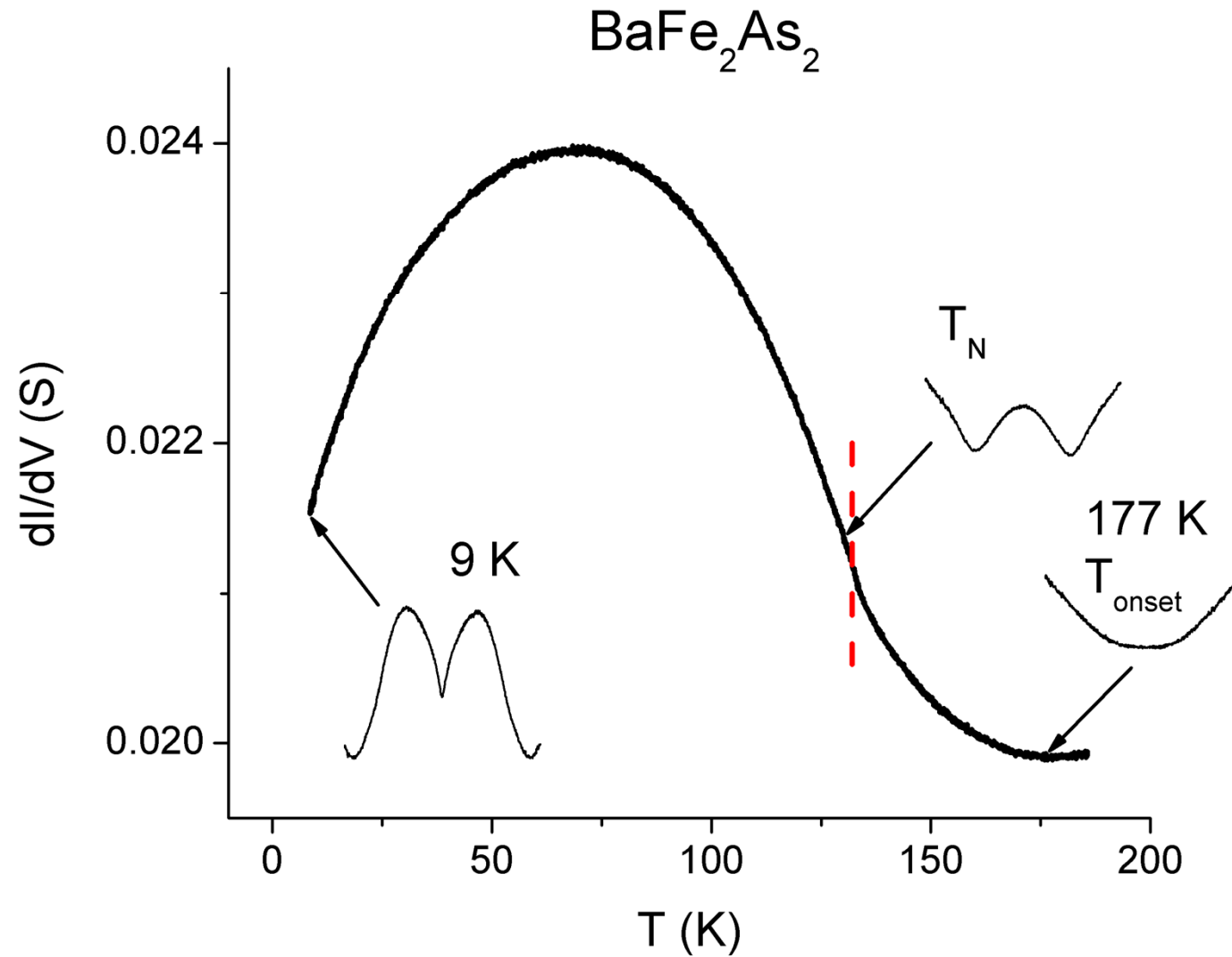
**This talk:** Enhancement at high-T in Co:BaFe<sub>2</sub>As<sub>2</sub> and FeTeSe.

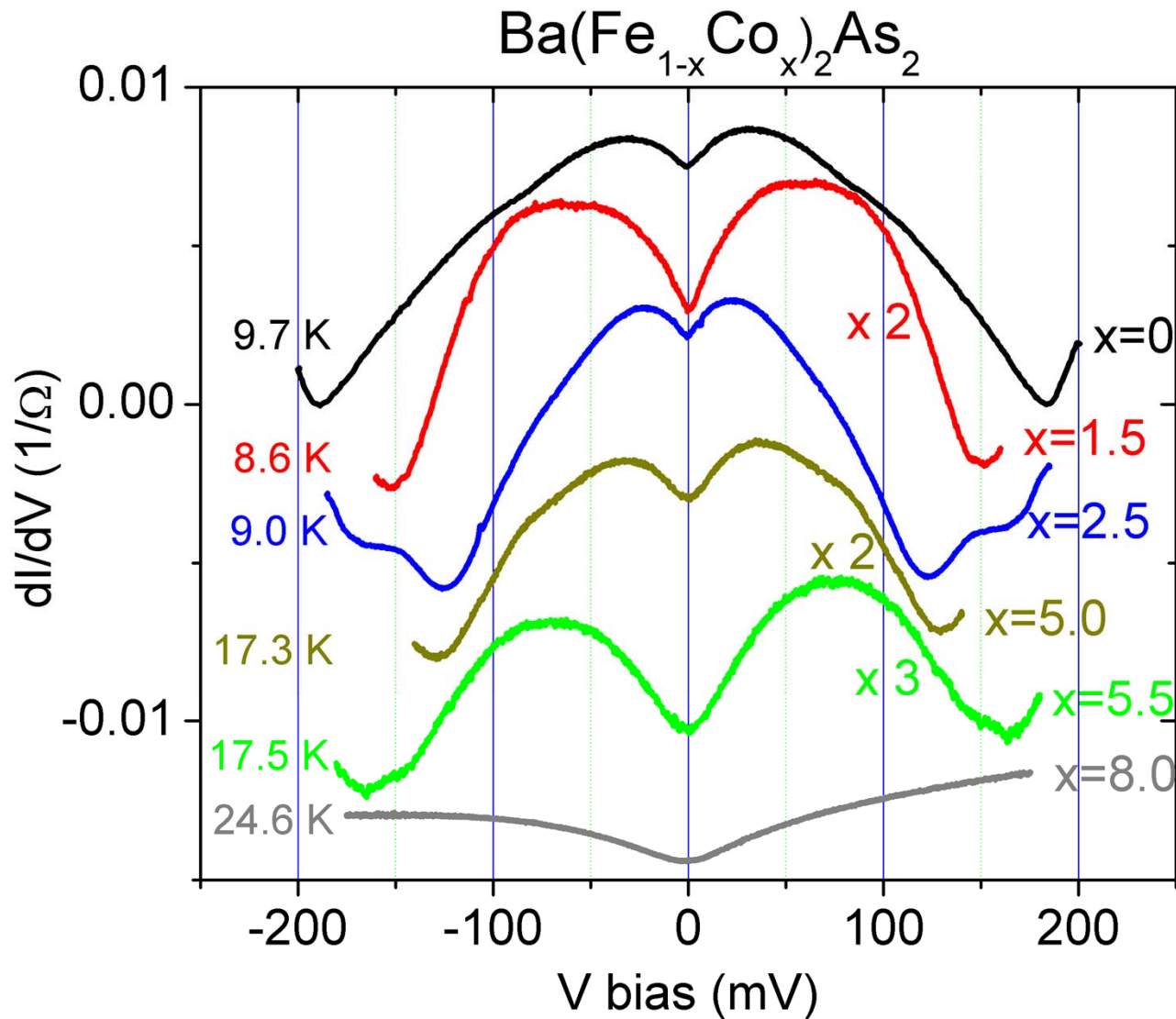
*Thank You !*



# $T_{\text{onset}}$ reflected in zero bias conductance

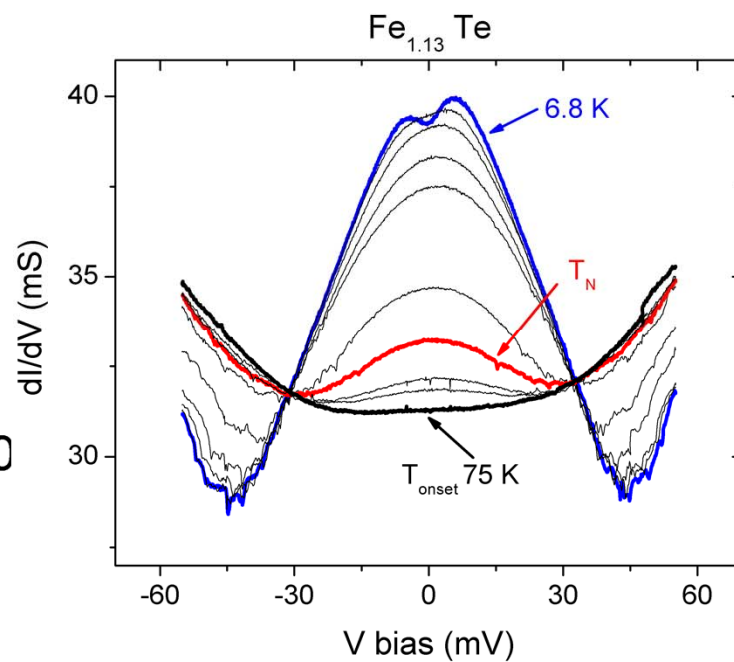
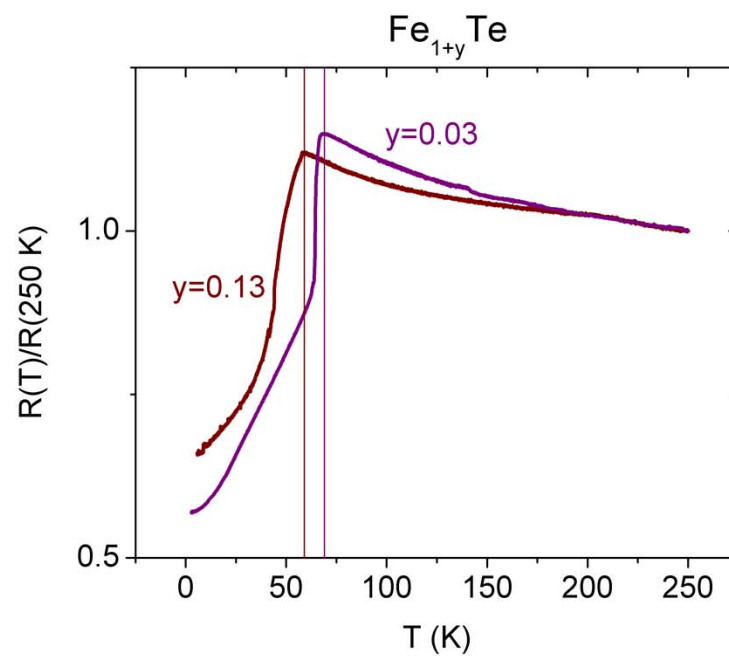
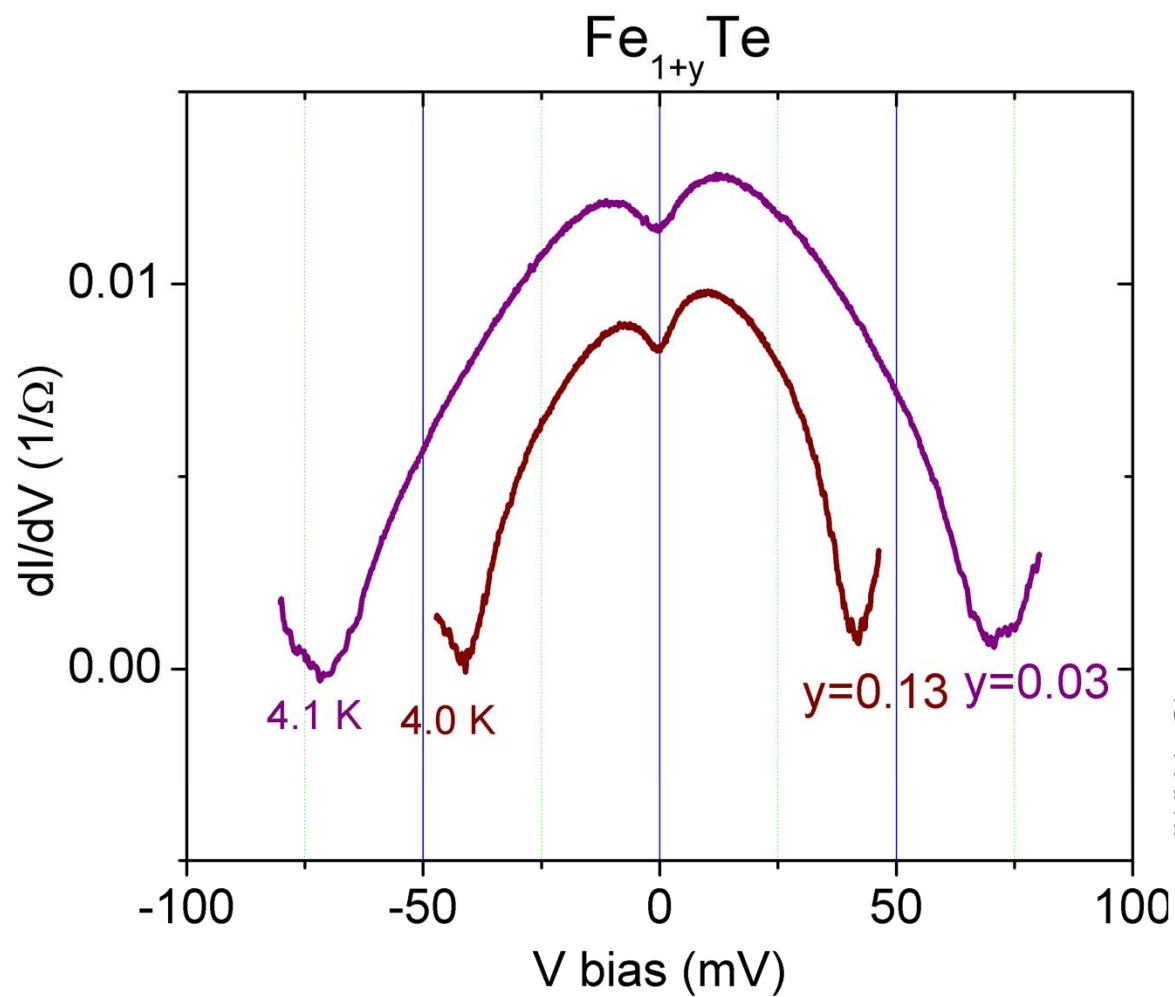
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Similar spectra observed when Co doping is low enough for magnetic order to exist (underdoped regime)

$\text{Fe}_{1+y}\text{Te}$  shows similar curves



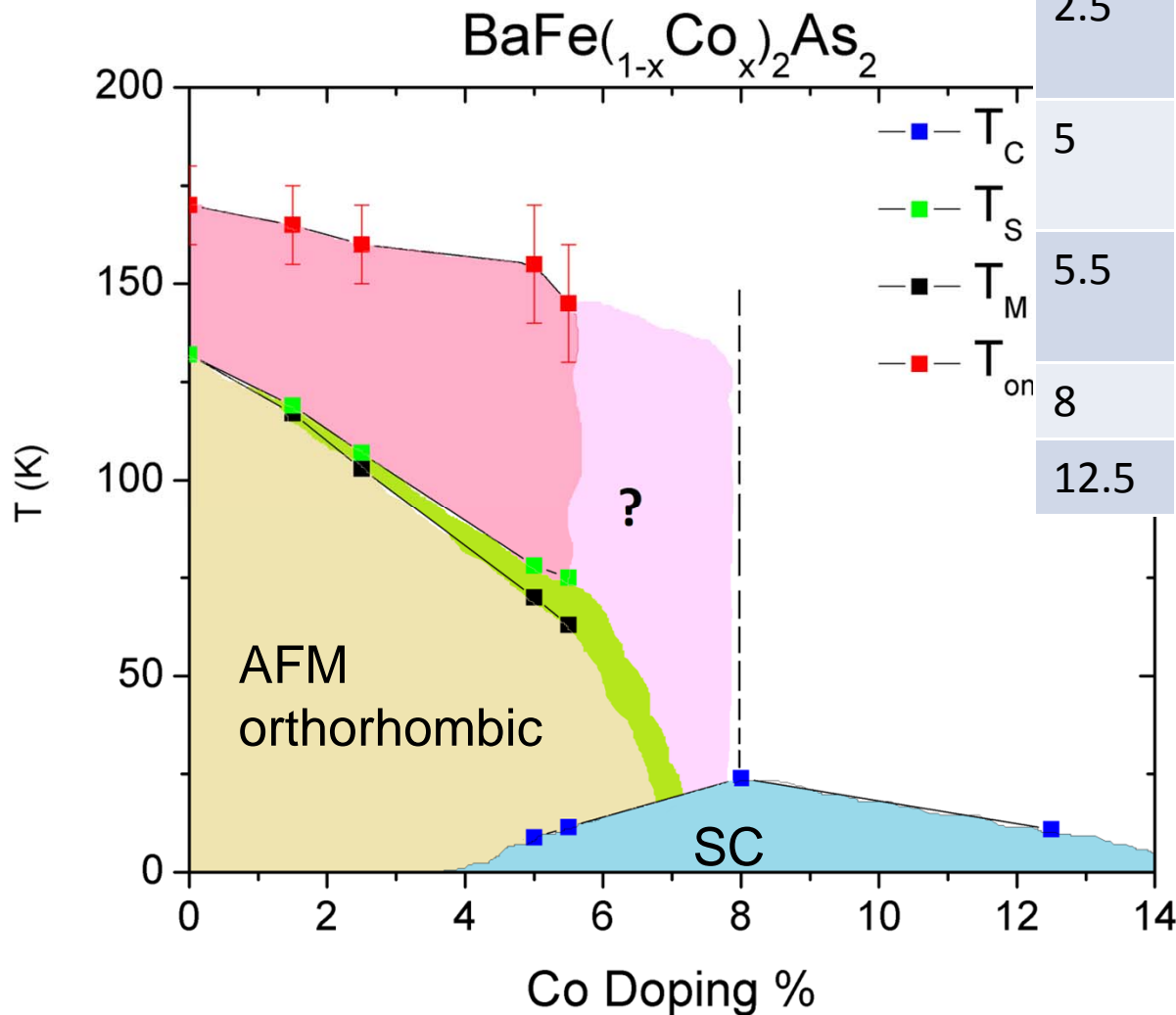
## Other experimental techniques that have observed signals above $T_S$ :

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- **ARPES:** Splitting between the  $d_{xz}$  and  $d_{yz}$  bands that develops above the magnetic transition temperature. Yi et al. arXiv:1011.0050v1 (to be published PNAS)
- **Inelastic Neutron Scattering:** Anisotropic high energy spin excitations in the paramagnetic phase. Harriger et al. arXiv:1011.3771v1
- **Resistivity:** In-plane resistive anisotropy above  $T_S$ . *Chu et al. Science* 329, 824 (2010);
- **Optical Conductivity:** Anisotropic charge dynamics above  $T_S$ . Dusza et al. arXiv:1007.2543v1

These signals are attributed to unequal occupation of the  $d_{xz}$  and  $d_{yz}$  bands, leading to orbital ordering above  $T_M$ . The unequal occupation is speculated to occur due to spin excitations or some sort of instability preferring one band over the other.

# Modified Phase Diagram & Conclusion



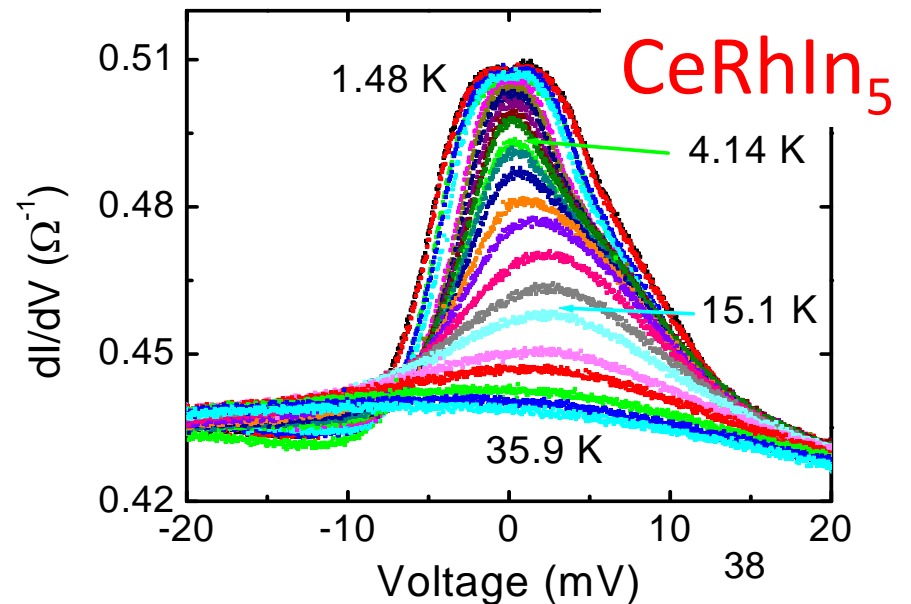
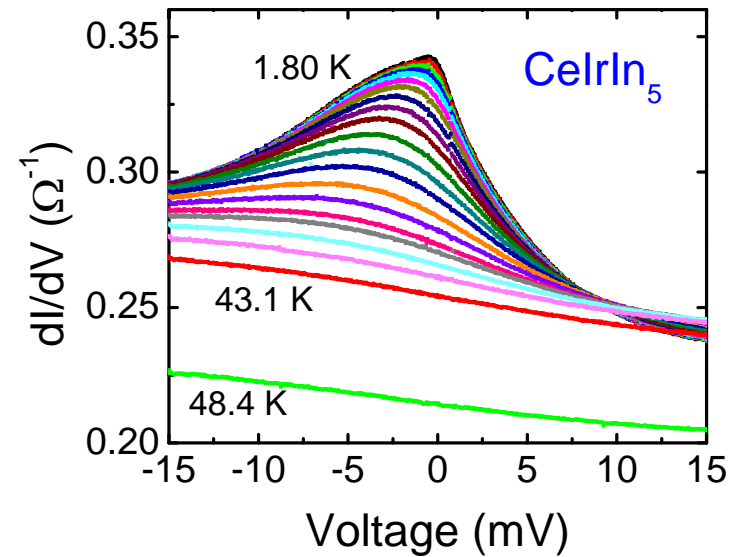
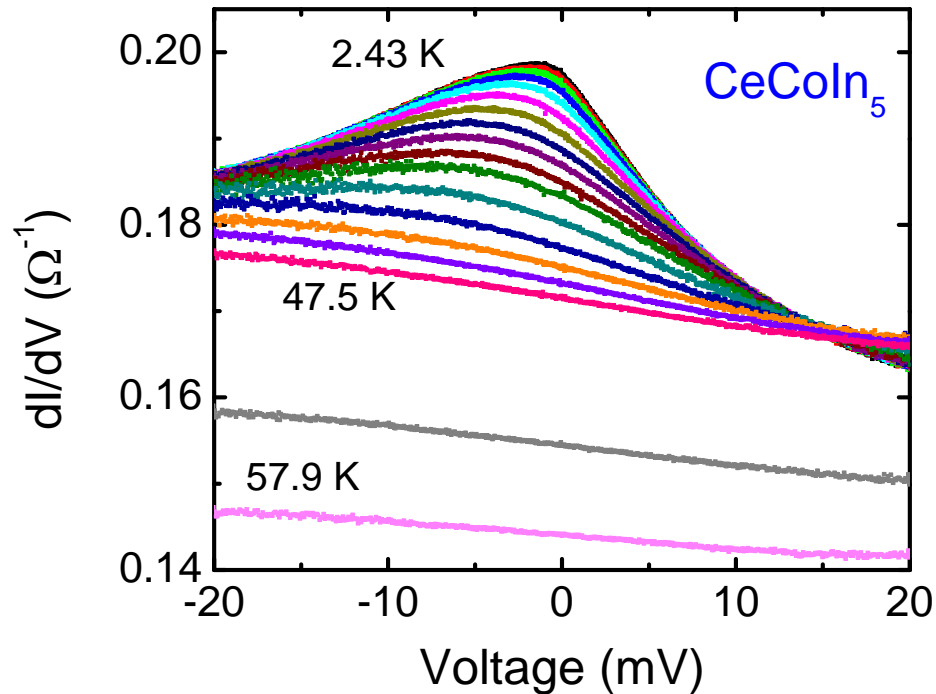
% Co	$T_N$	$T_S$	$T_{onset}$	$T_{c\_mid}$
0	132 K	132 K	$170 \pm 10$ K	-
1.5	117 K	119 K	$165 \pm 10$ K	-
2.5	103 K	107 K	$160 \pm 10$ K	-
5	70 K	78 K	$155 \pm 15$ K	8.9 K
5.5	63 K	75 K	$145 \pm 15$ K	11.5 K
8	-	-	-	24 K
12.5	-	-	-	11 K

• PCS is detecting a signal only for samples with magnetism.

• However, the signal survives well above  $T_N$ .

• We speculate that orbital ordering might be responsible for our conductance spectra.

# Antiferromagnetism (& Kondo): $\text{CeMIn}_5$



- Asymmetry: robust & reproducible in pure and Hg- & Cd-doped 1-1-5.
- Co: asymmetry follows HF spectral weight qualitatively (two-fluid model, Nakatsuji-Pines-Fisk).
- Rh: enhancement due to AFM

# Quasiparticle Tunneling into a Kondo Lattice

PRL 103, 206402 (2009)

PHYSICAL REVIEW LETTERS

week ending  
13 NOVEMBER 2009

## Electron Cotunneling into a Kondo Lattice

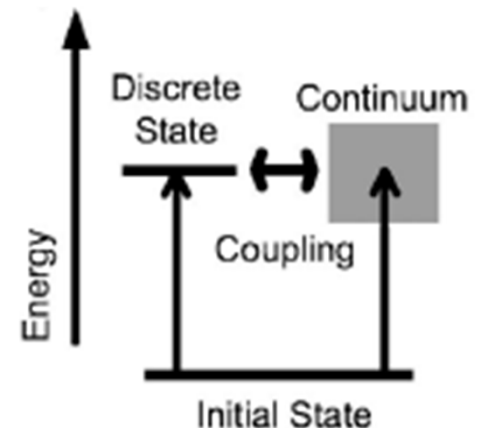
Marianna Maltseva, M. Dzero, and P. Coleman

Center for Materials Theory, Rutgers University, Piscataway, New Jersey 08854, USA

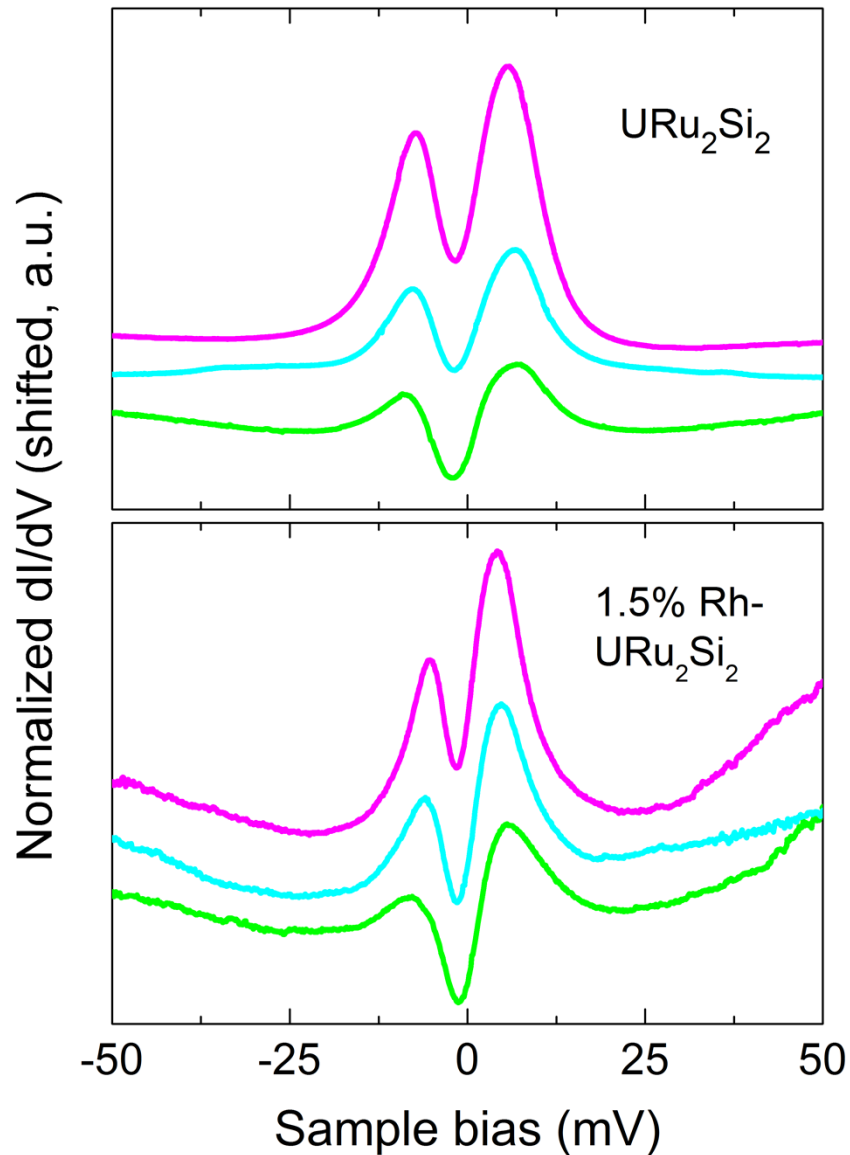
$$\left. \frac{dI}{dV} \right|_{FR} \propto \text{Im} \tilde{G}_{\psi}^{KL}(eV); \tilde{G}_{\psi}^{KL}(eV) = \left( 1 + \frac{q_F W}{eV - \lambda} \right)^2 \ln \left[ \frac{eV + D_1 - \frac{V^2}{eV - \lambda}}{eV - D_2 - \frac{V^2}{eV - \lambda}} \right] + \frac{2D/t_c^2}{eV - \lambda}$$

- $q_F$ : Fano asymmetry parameter ( $\equiv A/B$ ;  $A$  = probability for tunneling into heavy bands,  $B$  = into cond. band)
- $W = \pi N(0) V^2$ : width of the Kondo resonance
- $\lambda$ : renormalized  $f$ -level
- $-D_1, D_2$ : cond. band edges;  $2D = D_1 + D_2$ : band width
- If  $D_1 = D_2$ ,  $\Delta_{\text{hyb}} = 2V^2 / D$  (hybridization gap)
- $t_c$ : amplitude of direct tunneling into cond. band

Fano resonance!



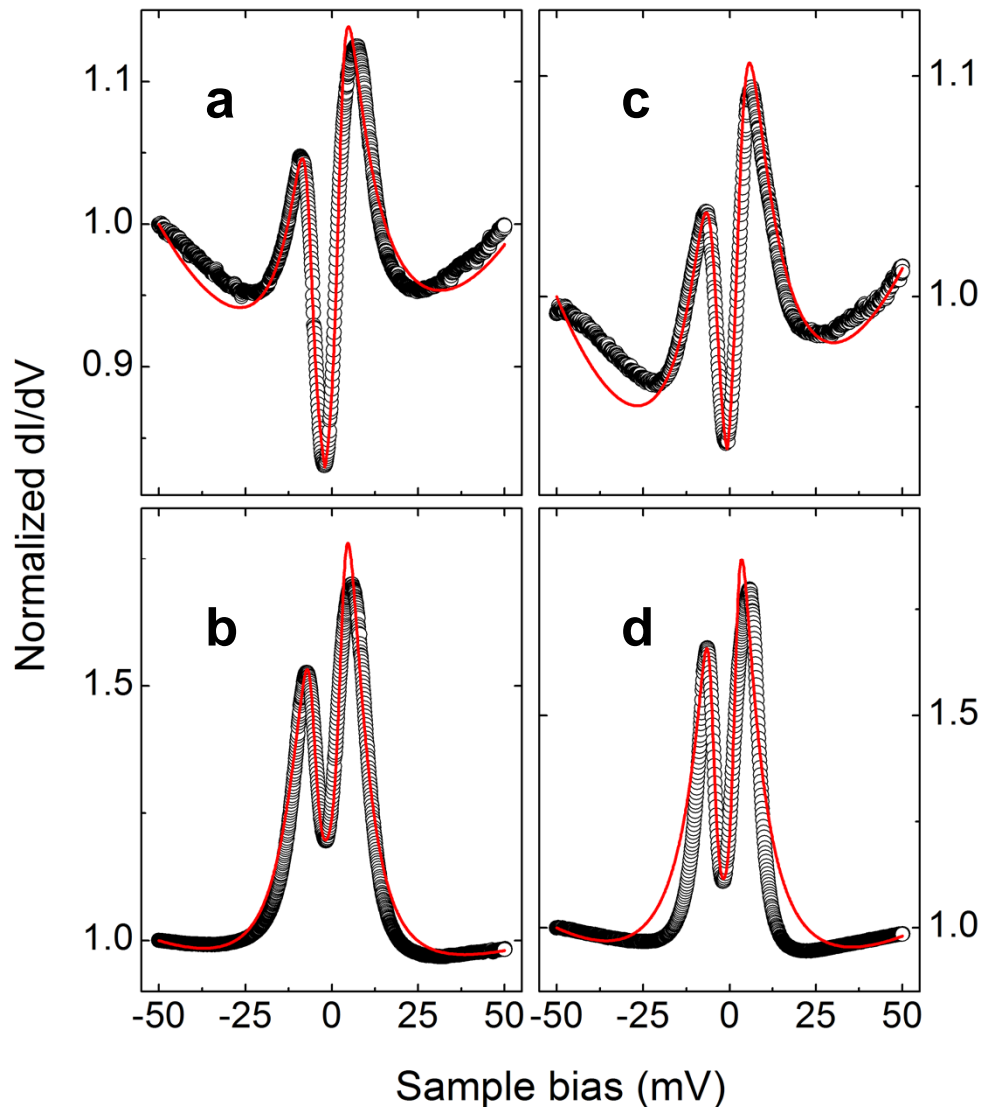
# Conjecture on a Fano Resonance



- Data taken from different junctions, showing a systematic variation.
- Asymmetric double-peak structure is reproducibly observed.
- Positive-bias conductance peak is always higher ( $\Rightarrow q_F > 0$ ).
- $V_{\min} = -3 \sim -0.5 \text{ mV} < 0 @ T \ll T_{\text{HO}}$   
 $\Rightarrow$  These observations lead us to conjecture on a **Fano resonance in a Kondo lattice**, as predicted by Maltseva-Dzero-Coleman (**PRL 2009**).
- Interference between channels into the hybridized heavy bands ( $A$ ) and the conduction band ( $B$ ).  $q_F \equiv A/B$ .



# Analysis Using a Fano Resonance Model



$$\frac{dI}{dV} = \frac{dI}{dV}\bigg|_{FR} + \omega \cdot \frac{dI}{dV}\bigg|_{bg}$$

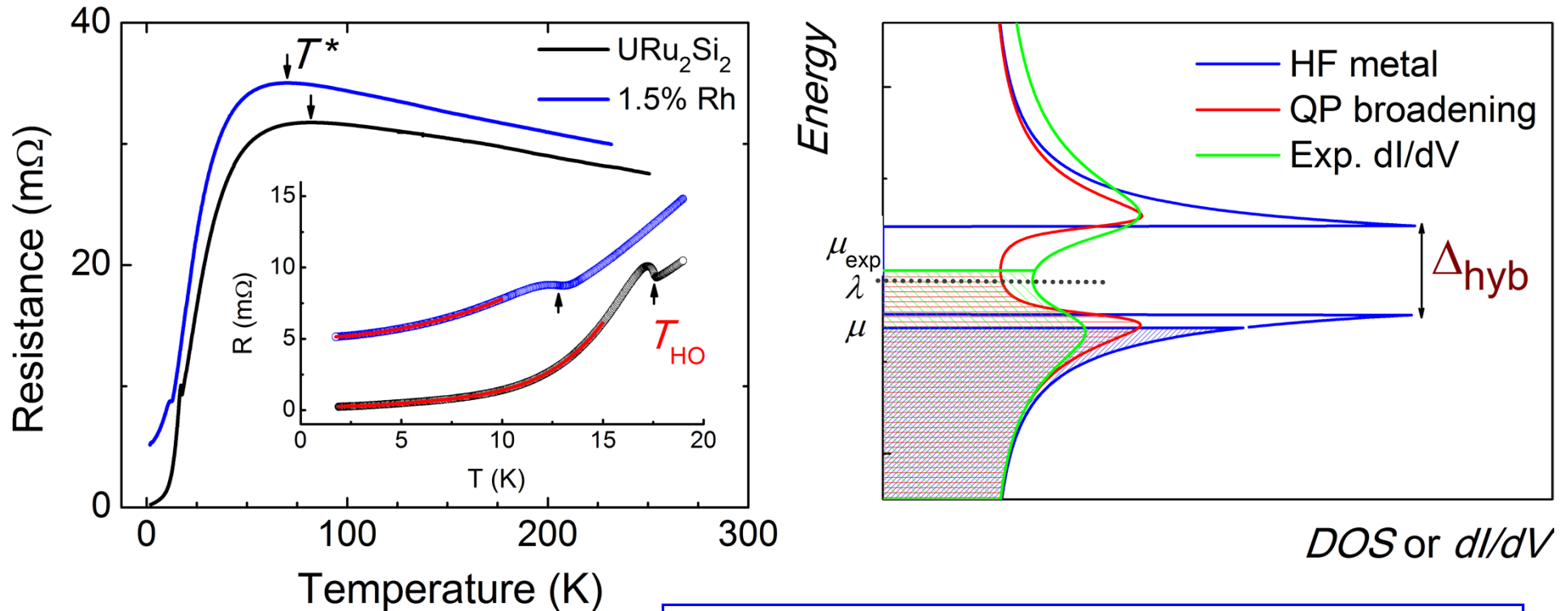
Fano resonance      Background  
(Maltseva et al., 2009)

- Assume a parabolic background
- Energy-dep. quasiparticle broadening due to correlation effects,  $\gamma(E)$  (Wölfle et al., PRL, 2010)

Fig. #	a	b	c	d
T (K)	2.07	3.13	4.35	2.40
$R_J$ (W)	16.7	19.1	51.0	39.0
$q_F$	10	11	11	13
$\Delta_{hyb}$ (meV)	12.1	11.7	14.2	10.9
$V$ (meV)	41.4	40.7	44.8	39.0
$\lambda$ (meV)	-2.0	-0.7	-1.2	-1.6

- Average  $\Delta_{hyb} = 13$  meV, consistent with recent optical spectroscopy results by Levallois et al. (arXiv:1007.0538)

# Relation to Gaps from Other Measurements



$$R = R_0 + aT^2 + b(T / \Delta)[1 + 2T / \Delta] \exp(-\Delta / T)$$

- Fitting gives rise to  $\Delta = 6.7 \text{ meV} \approx \Delta_{\text{hyb}}/2$ .
  - 1.5% Rh-doped ( $T_{\text{HO}} = 12.8 \text{ K}$ ):  $\Delta = 4.7 \text{ meV}$ ,  $\Delta_{\text{hyb}} = 10 \text{ meV}$ .  $\Rightarrow \Delta \approx \Delta_{\text{hyb}}/2$ .
  - Finite conductance within  $\Delta_{\text{hyb}}$  indicates **finite DOS** (e.g., due to correlation effects) with the chemical potential close to the gap center.
- $\Rightarrow \Delta$  is approximately half of  $\Delta_{\text{hyb}}$ .