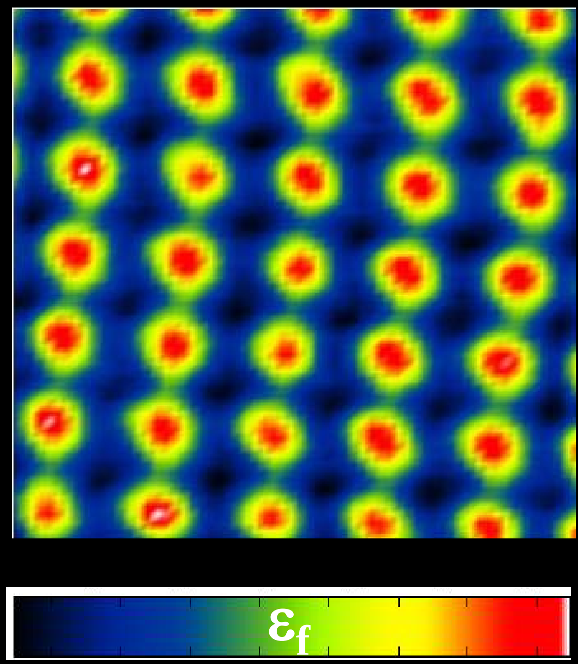
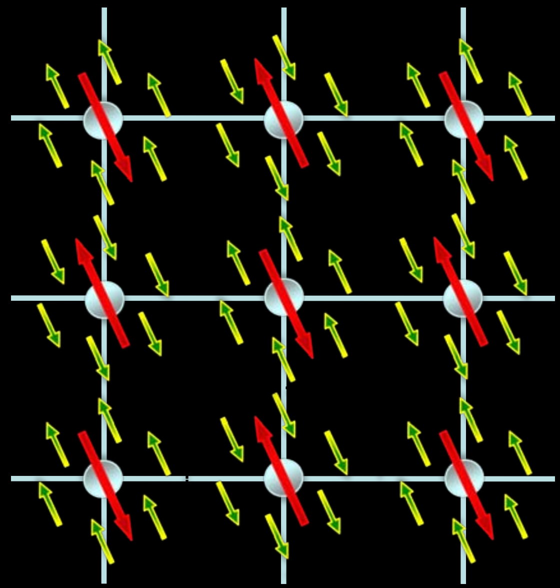
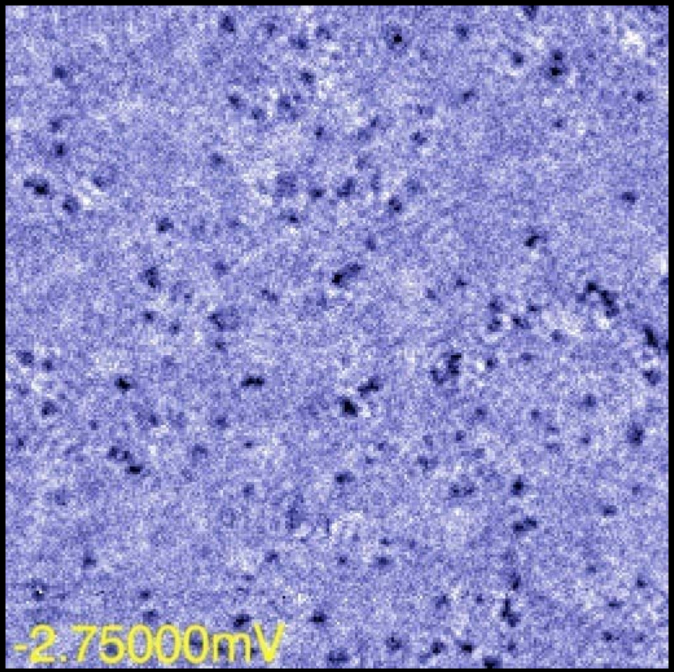
Emergence of the Hidden Order State from the Fano Lattice Electronic Structure of the Heavy-Fermion Material URu_2Si_2





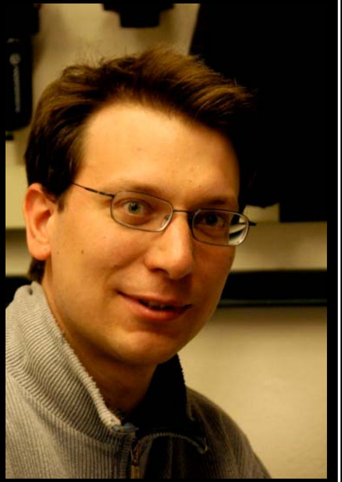


J.C. Séamus Davis

BROOKHAVEN NATIONAL LABORATORY
UBC

Cornell/McMaster URu_2Si_2 Team

Prof. Graeme Luke
McMaster



Dr. Peter Wahl
Cornell/MPI Stuttgart

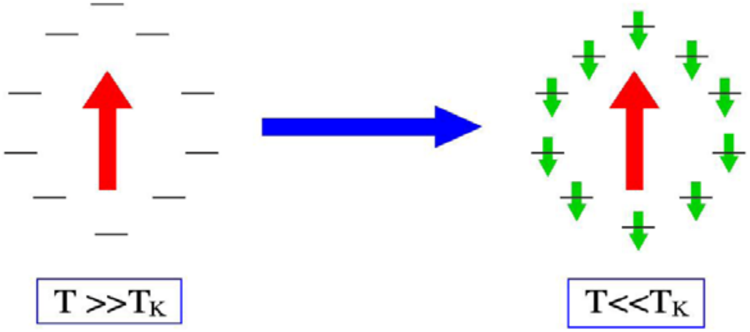
Mohammad Hamidian
Cornell / BNL

Dr. Andy Schmidt
Cornell / BNL

Kondo Lattice & Heavy Fermions

Kondo Effect

Kondo

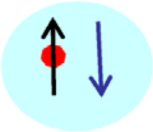


Wilson

T_K: characteristic Kondo temperature

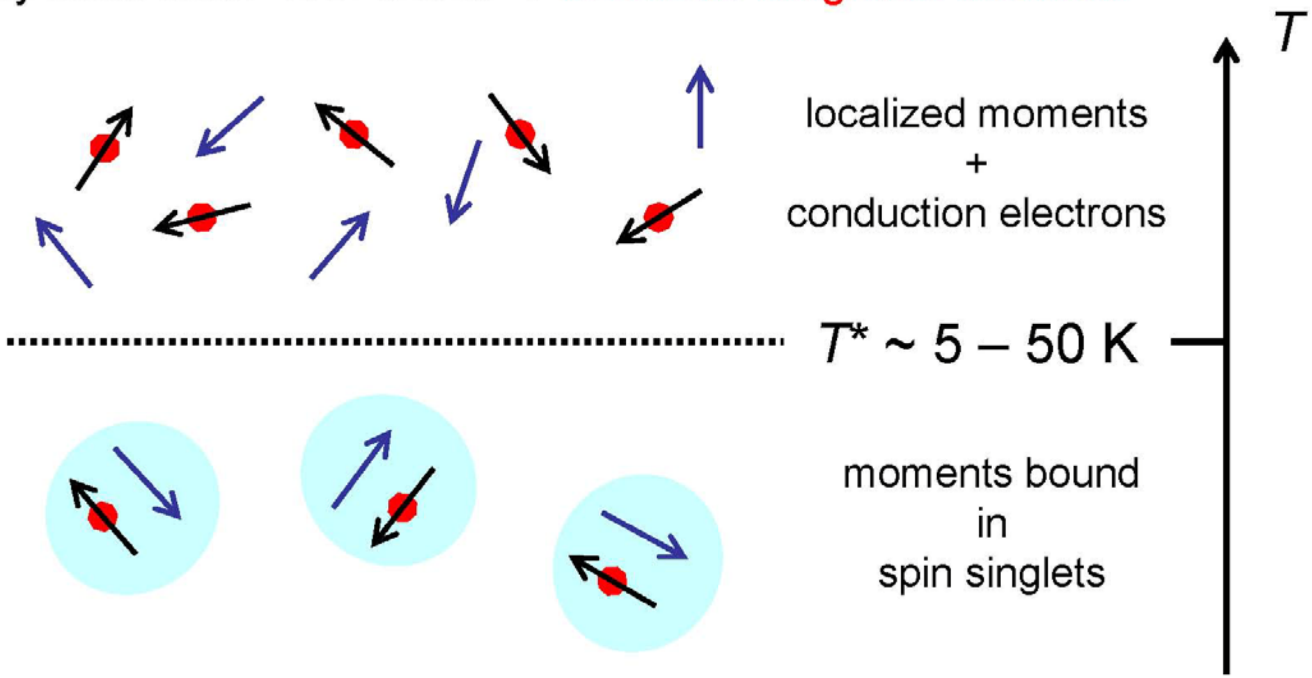
$$T_K \propto \exp(-1/\rho J)$$

Below T_K impurity spin is progressively screened: Kondo singlet

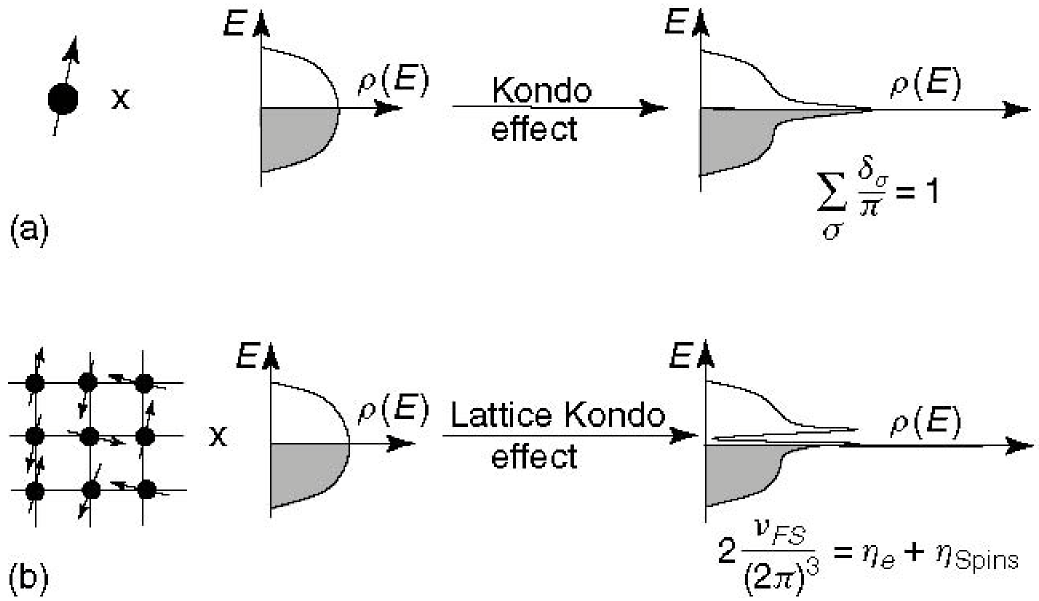


Heavy Fermion Effects in f-electron Lattices

- Lattice of certain *f*-electrons (most Ce, Yb or U) in metallic environment
- La^{3+}: $4f^0$, Ce^{3+}: $4f^1$ ($J = 5/2$), Yb^{3+}: $4f^{13}$ ($J = 7/2$)
- partially filled inner 4f/5f shells → localized magnetic moment



Kondo Impurity & Kondo Lattice

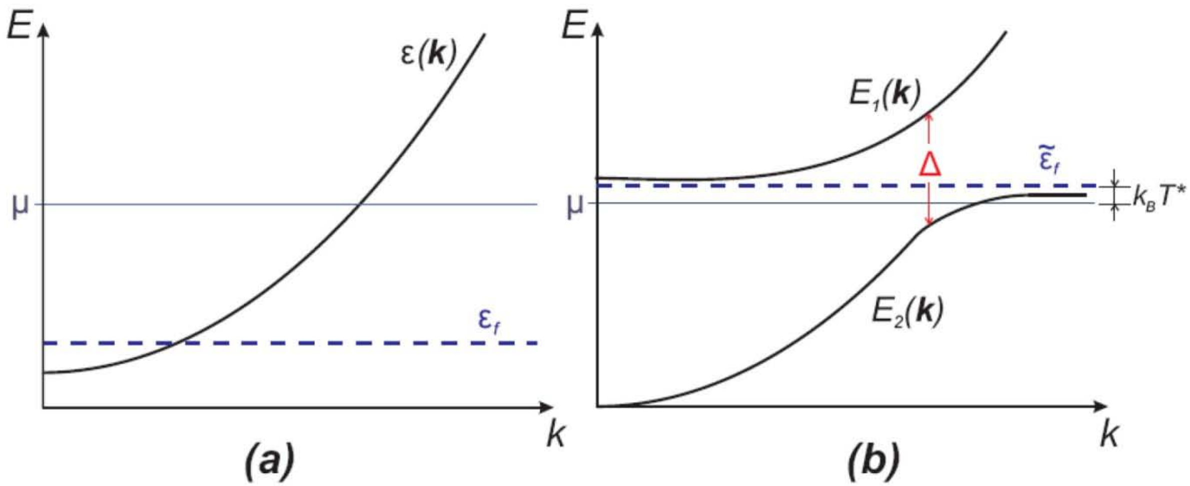


Interactions bring f level close to E=0 and result in a d-f hybridization and a sharp DOS(E) resonance

Heavy Fermion Effects in Kondo Lattices

High temperature

Low temperature

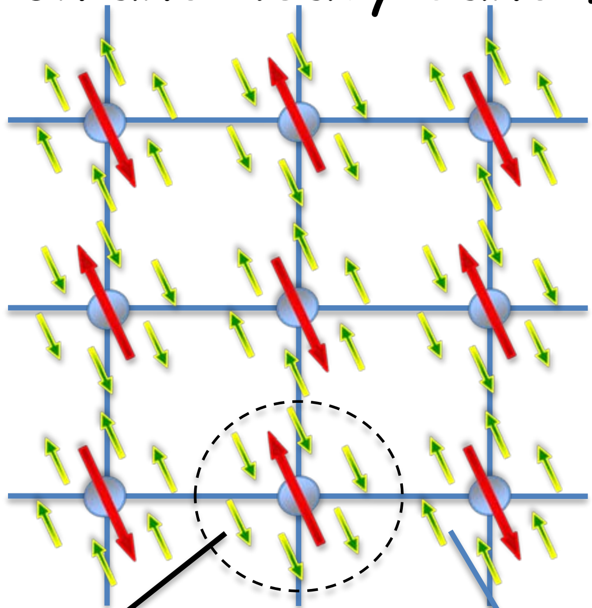


$$\varepsilon_k^{\pm} = \frac{\varepsilon_k^f + \varepsilon_k \pm \sqrt{\left(\varepsilon_k^f + \varepsilon_k\right)^2 + 4\,|V_k\,|^2}}{2}$$

Challenge: atomically resolved image of d-f electron hybridization and heavy band formation ?

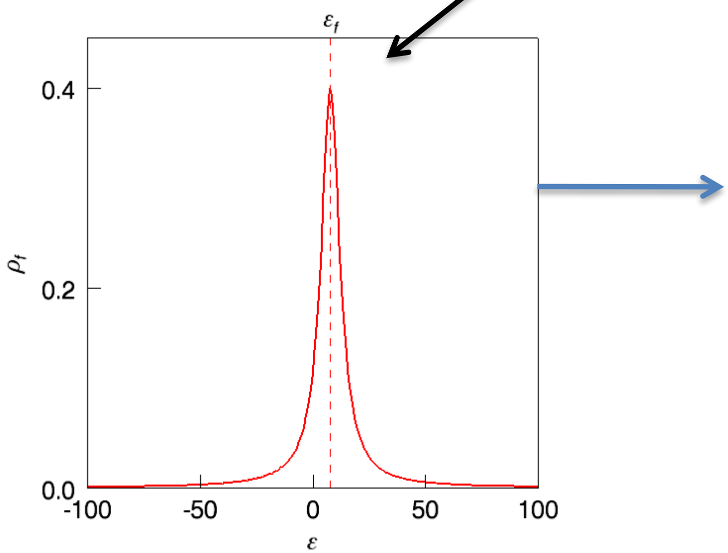
- Many-body resonance ε_f just above E=0

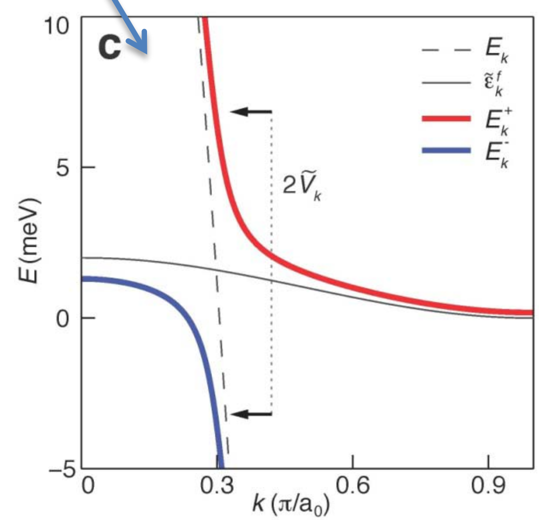
- Hybridization energy region Γ surrounding ε_f



- Light d-band beyond Γ from ε_f

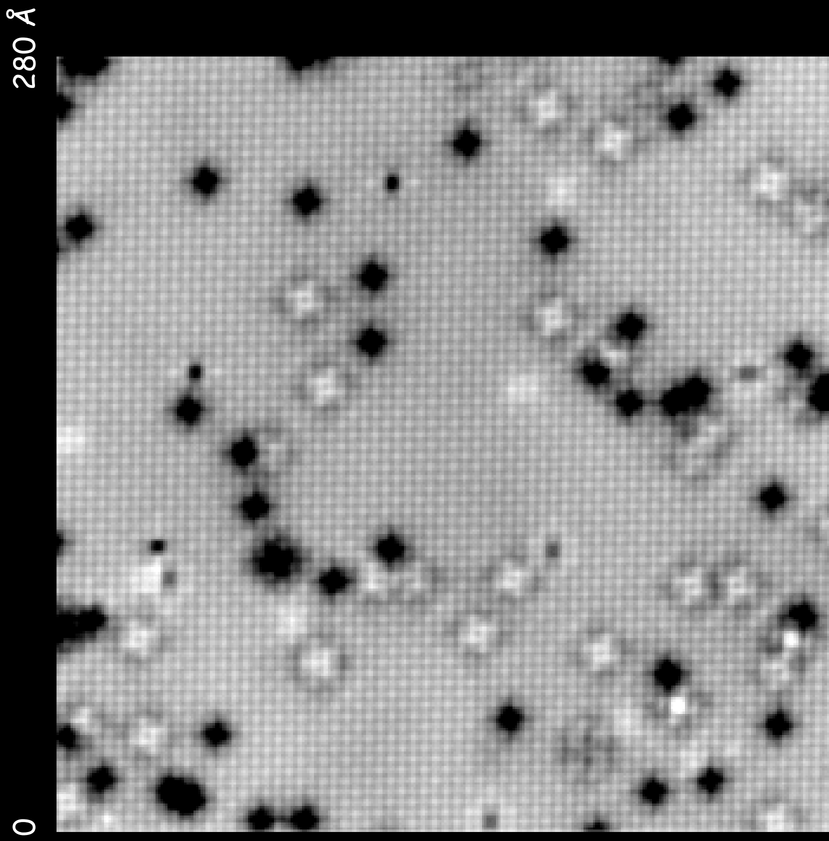
- High DOS and heavy f-band within Γ from ε_f

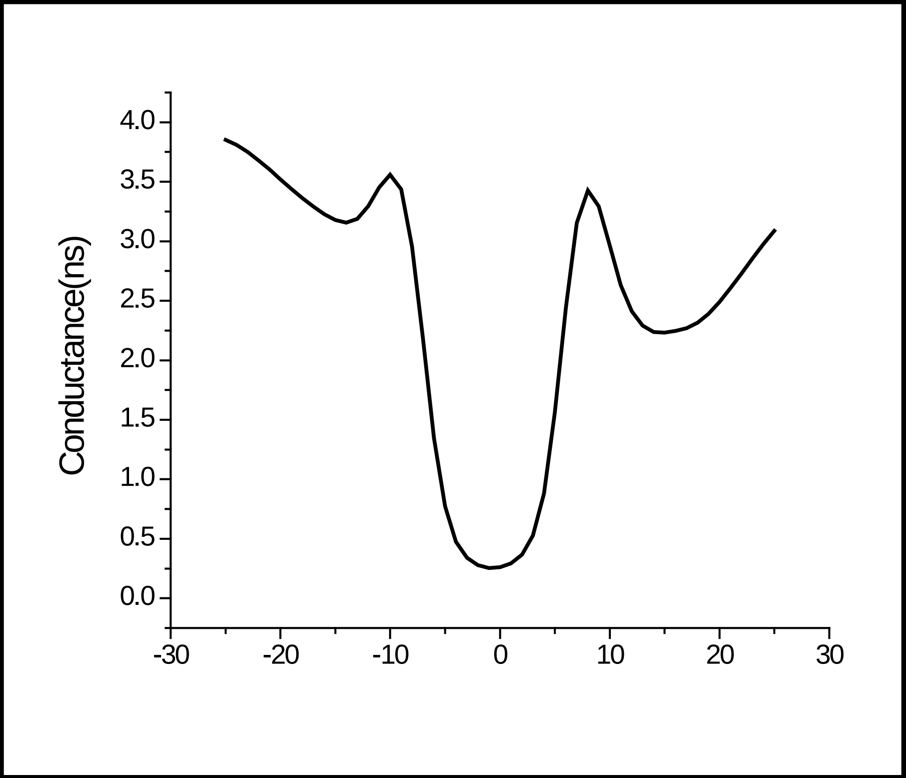




Heavy Fermion
Spectroscopic Imaging STM

Spectroscopic Imaging STM



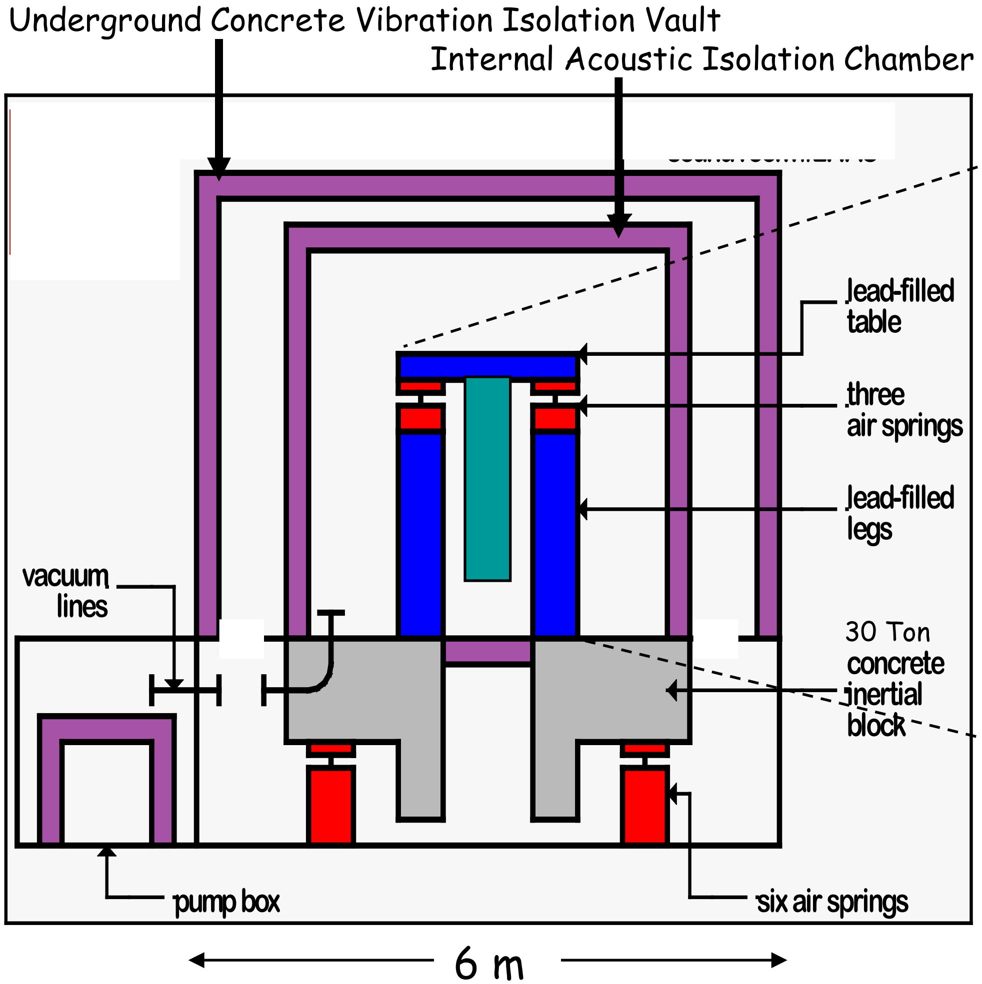


Spectroscopic Imaging STM Systems

Rev. Sci. Inst. 70, 1459 (1999).

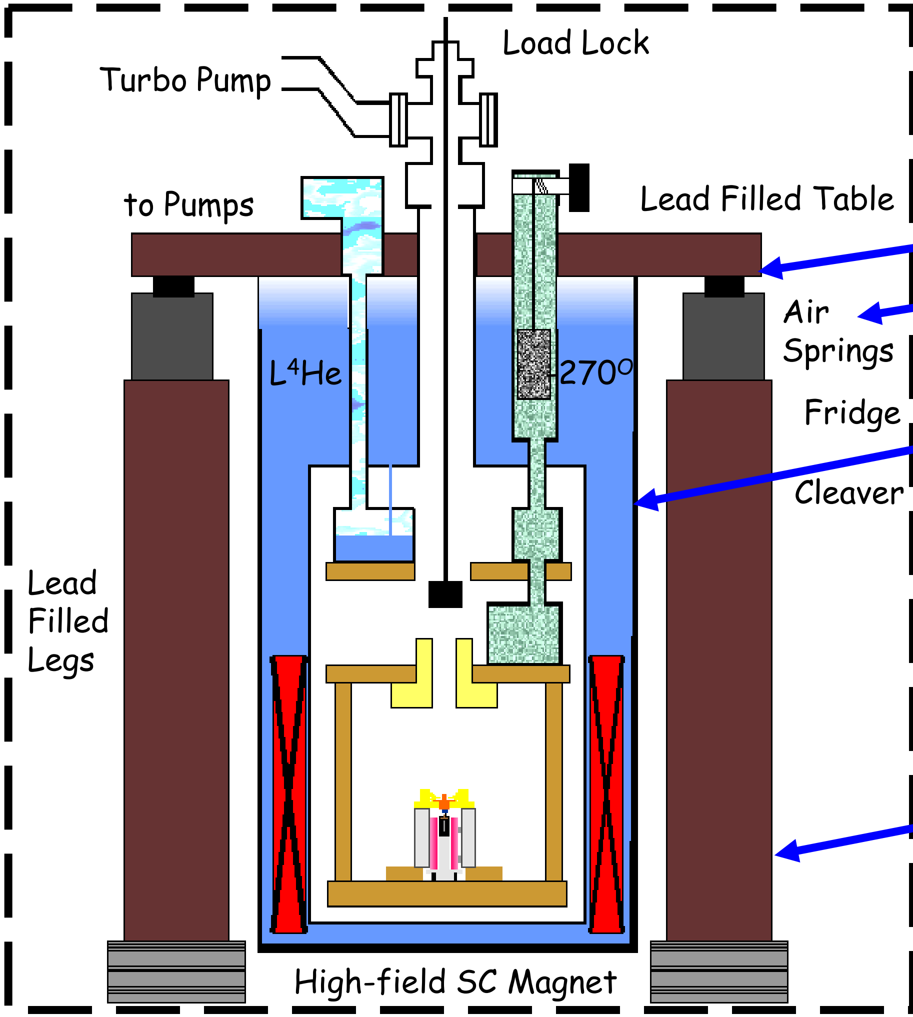
Ultra low vibration lab.

Ultra low vibration cryostat.



Spectroscopic Imaging STM Systems

Rev. Sci. Inst. 70, 1459 (1999).



Ultra low vibration cryostat.

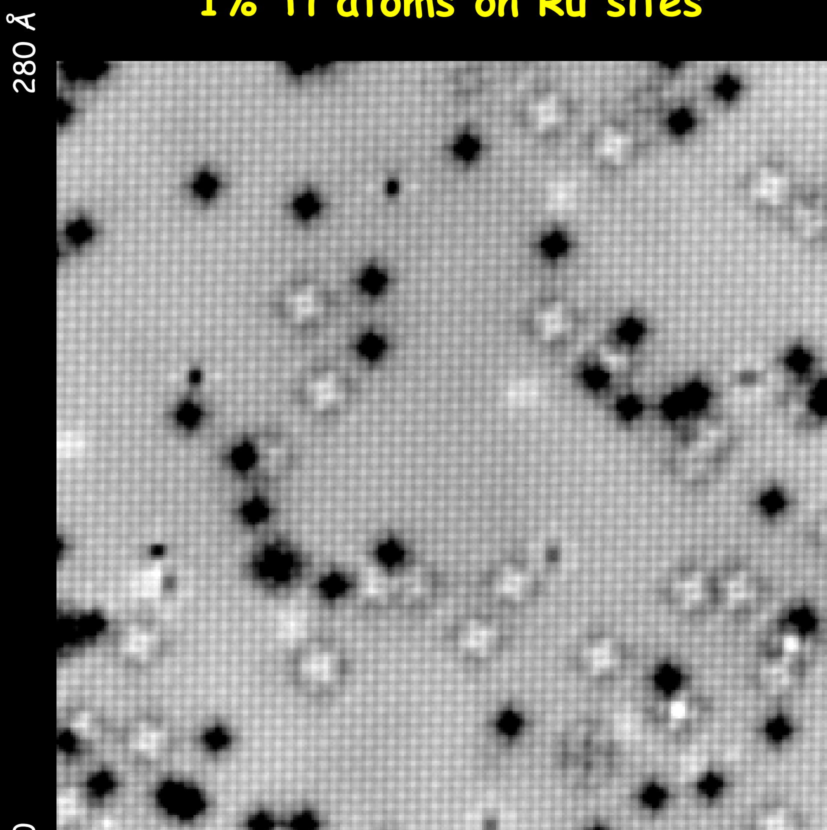
Spectroscopic Imaging STM Systems

Rev. Sci. Inst. 70, 1459 (1999).

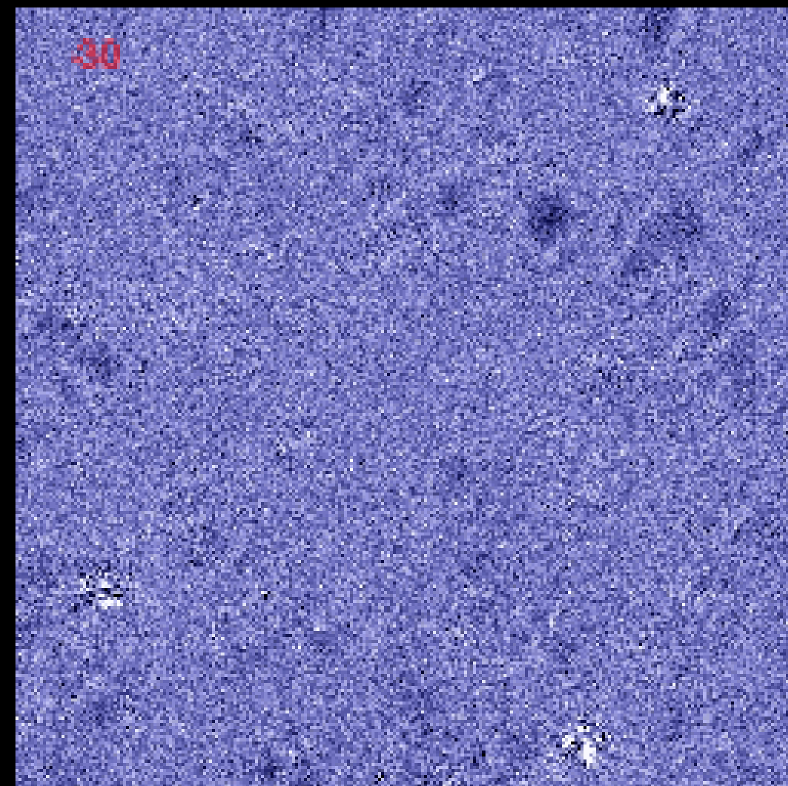
10 mK / 9 Tesla / SI-STM

Heavy Fermion QPI Example: $Sr_3Ru_2O_7$

1% Ti atoms on Ru sites



Spectroscopic Image $g(\vec{r}, E)$



***Nature Physics 5**, 800* (2009)

Heavy Fermion QPI Example: $Sr_3Ru_2O_7$

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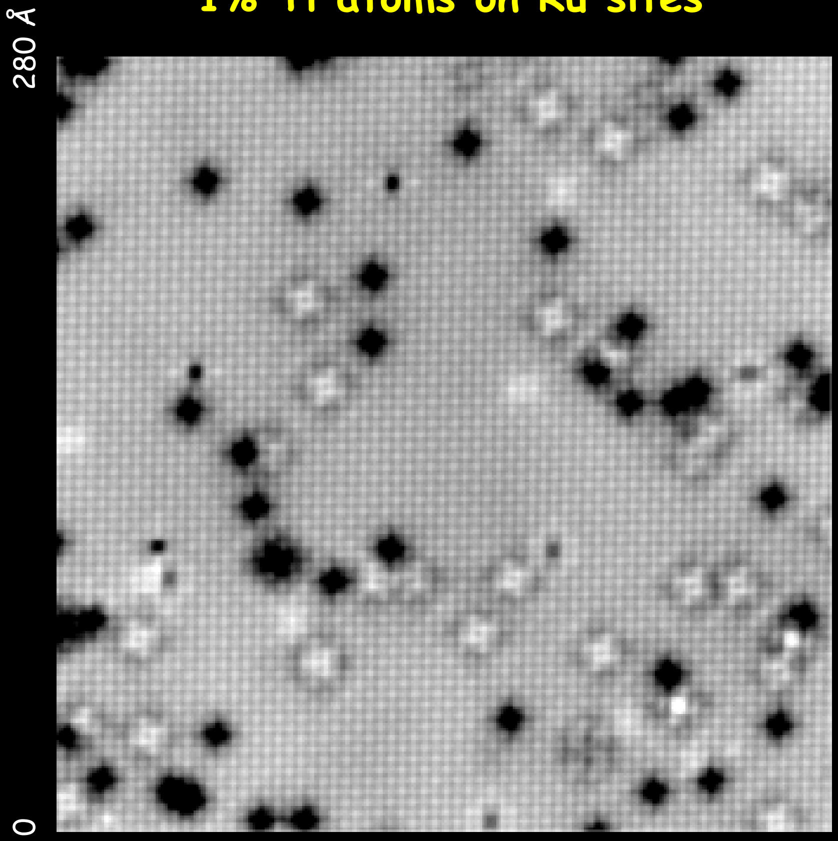
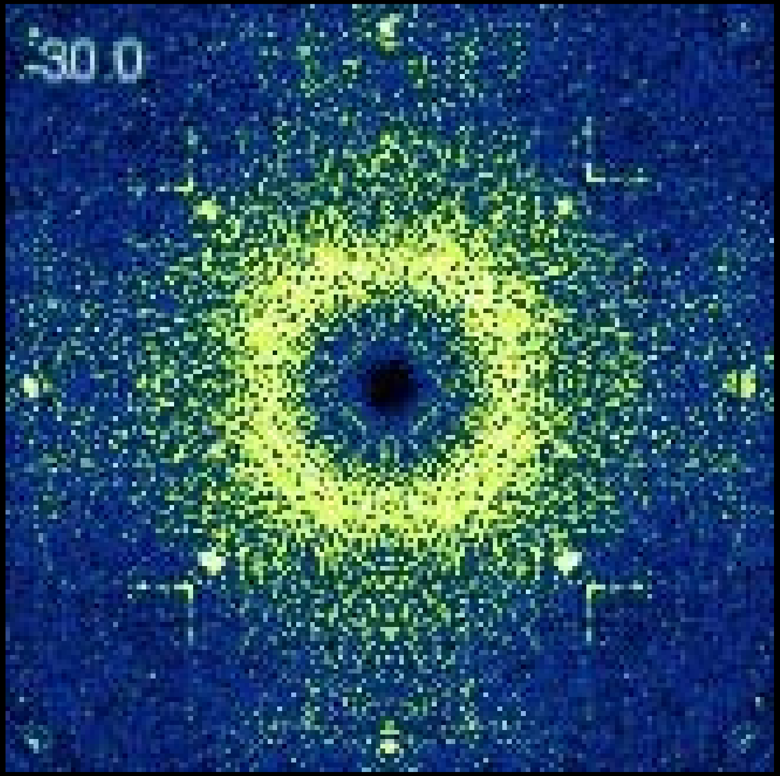
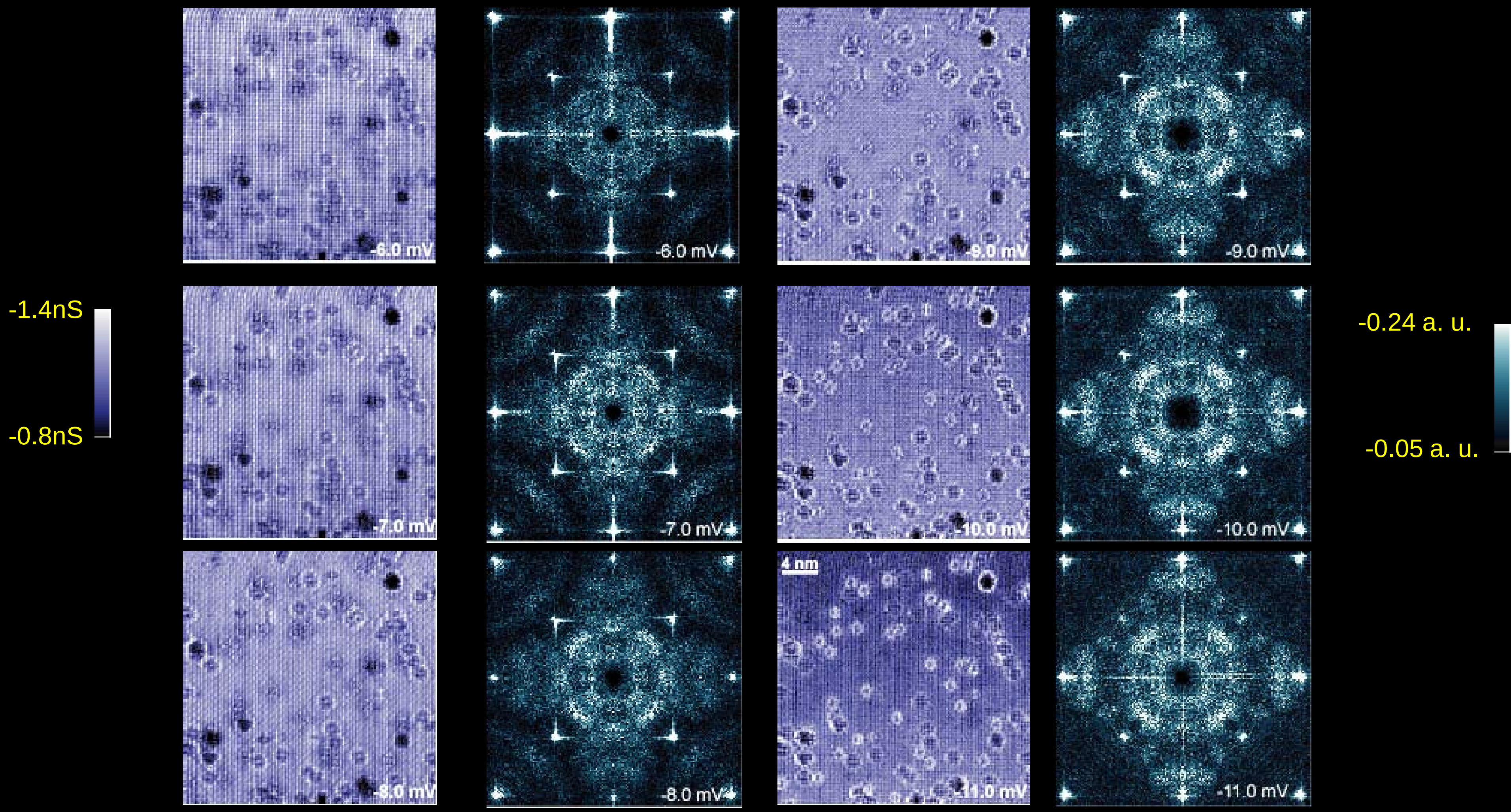


Spectroscopic Image $g(\vec{r}, E)$



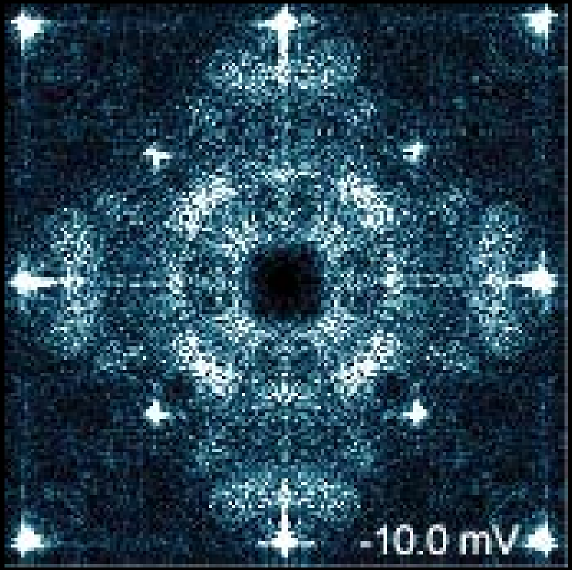
***Nature Physics* *5*, *800* (2009)**

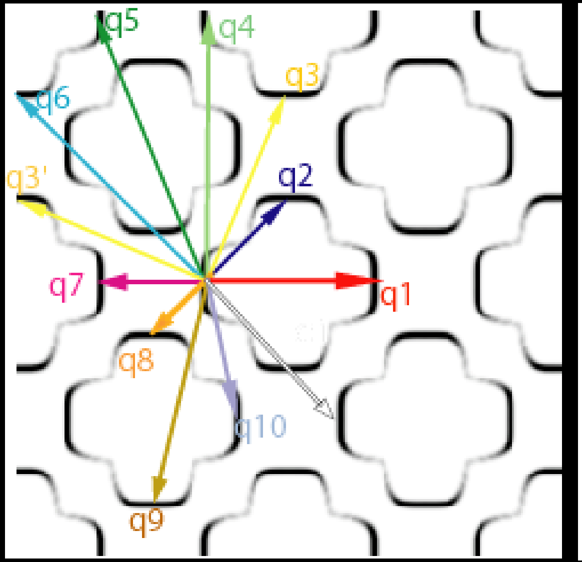
Heavy Fermion QPI Example: $Sr_3Ru_2O_7$

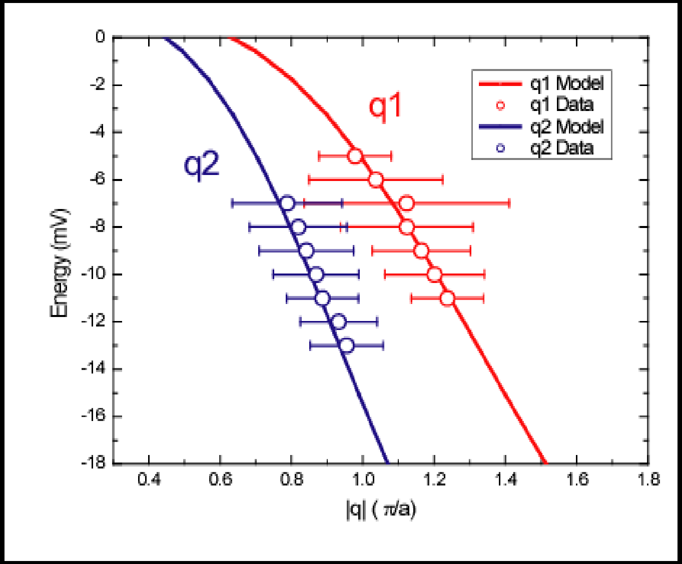


Nature Physics 5, 800 (2009)

QPI identification of heavy d-electron (α_2) band

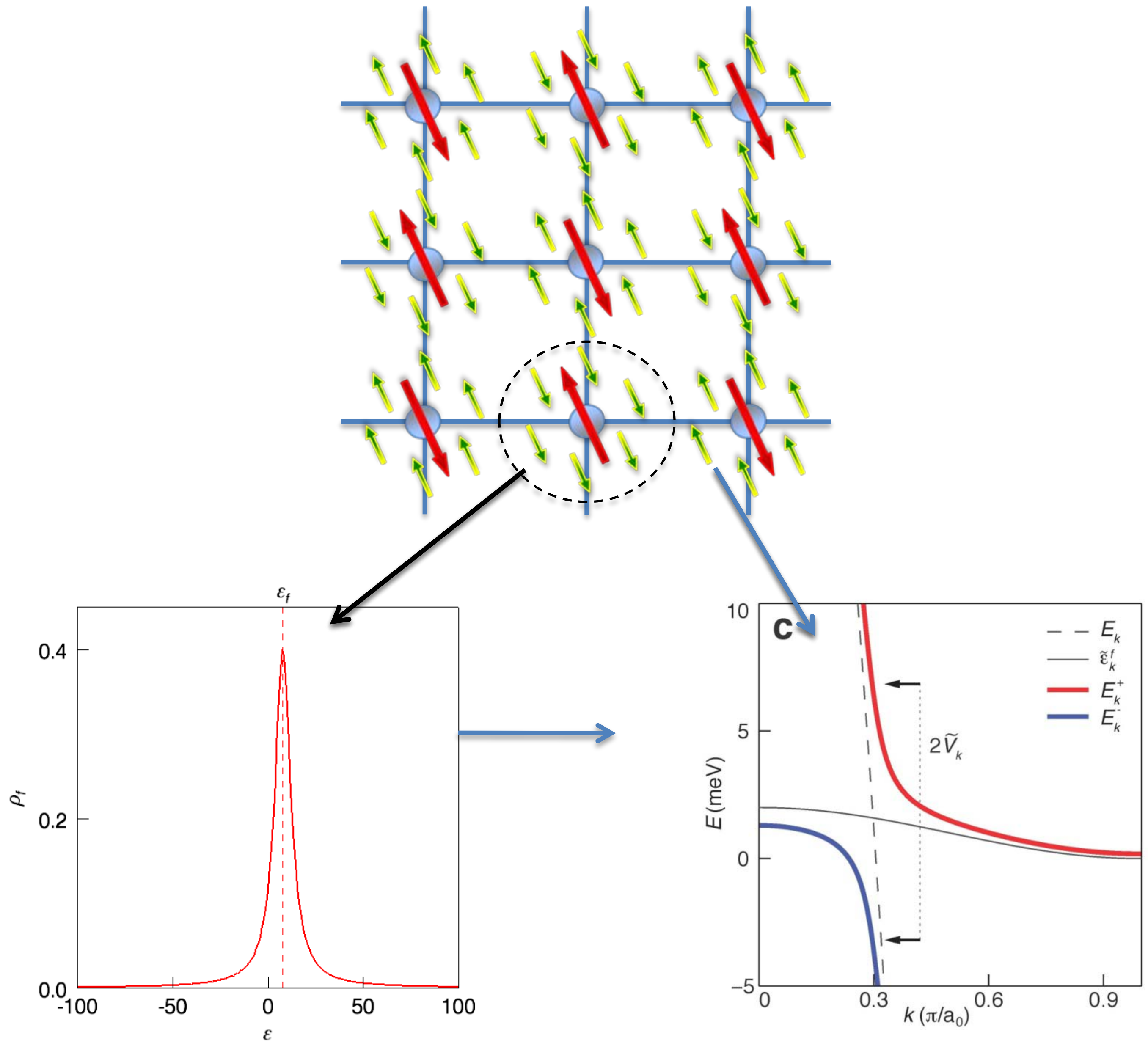






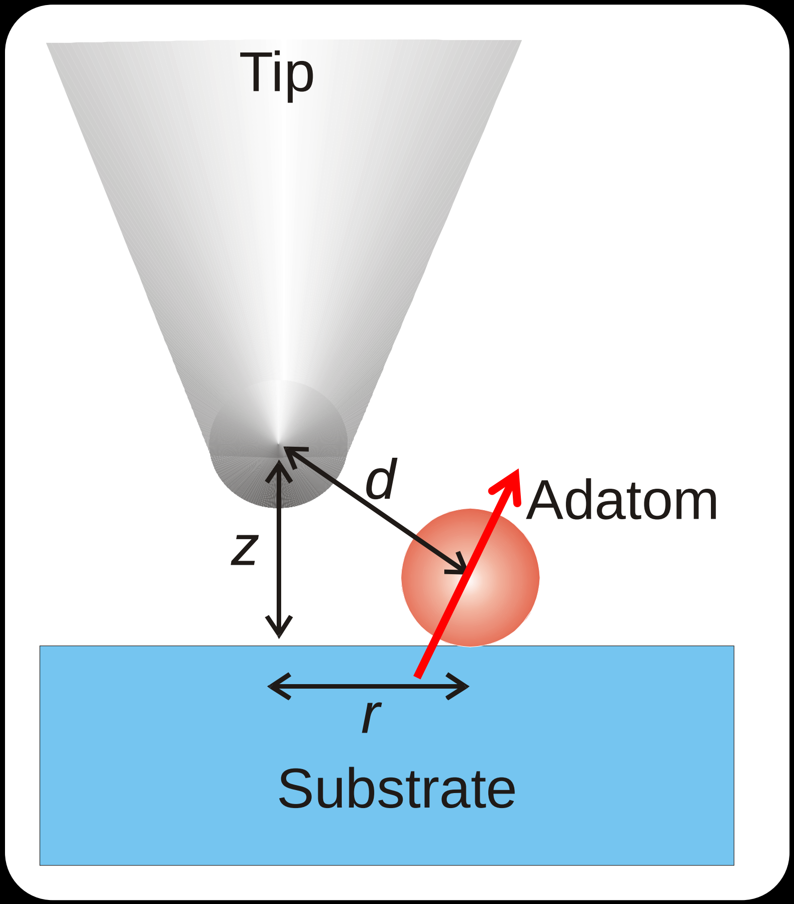
Nature Physics 5, 800 (2009)

Can we explore Kondo-Lattice Heavy Fermions similarly?



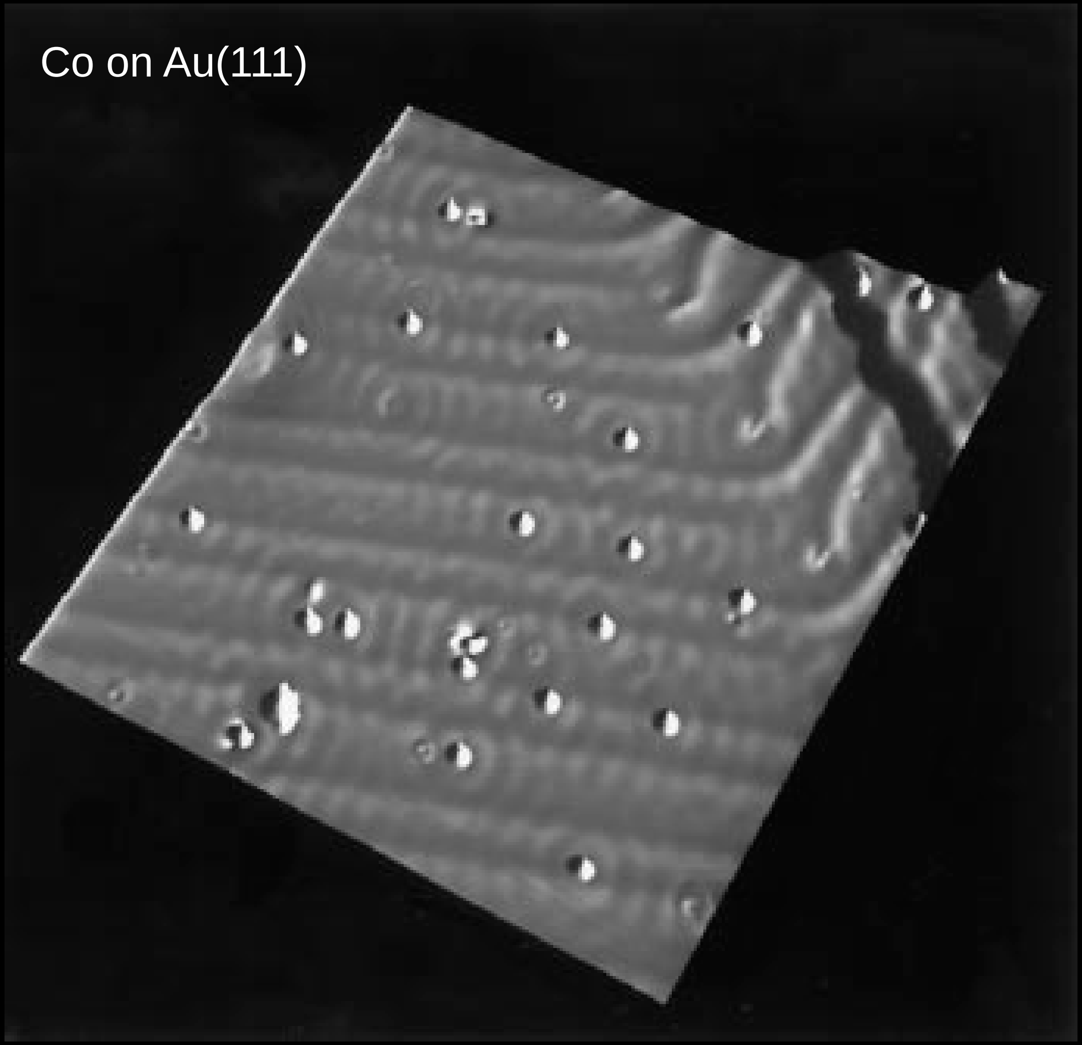
Single Adatom Kondo Effect

Single Magnetic Adatom Kondo Resonance



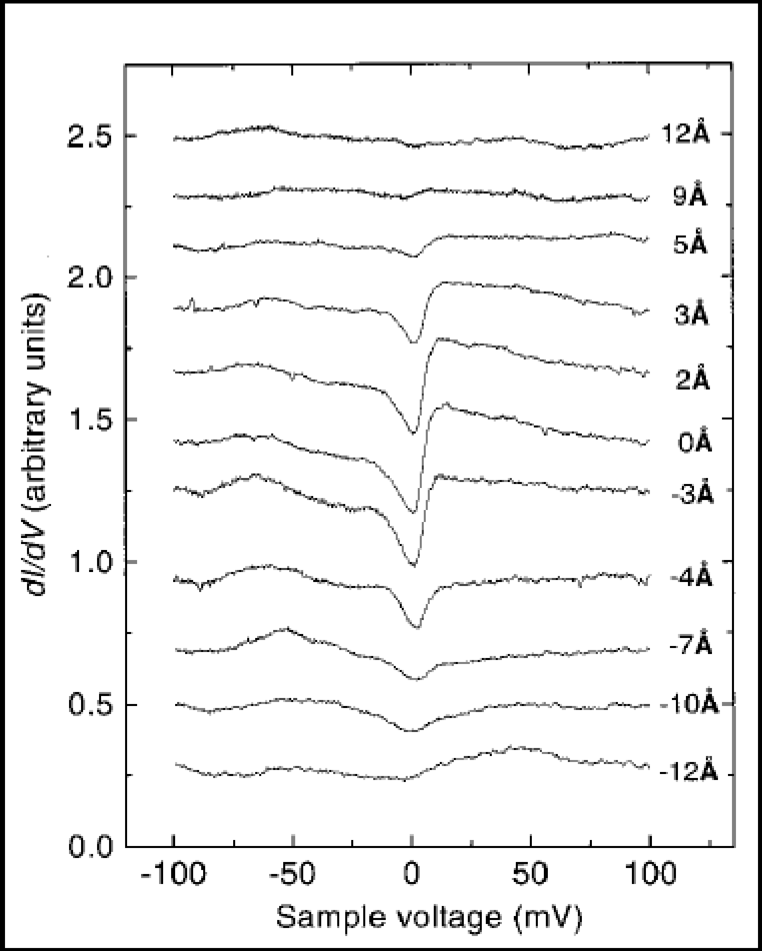
M. Plihal und J.W. Gadzuk, Phys. Rev. B 63, 085404 (2001)
O. Újsághy, J. Kroha, L. Szunyogh und A. Zawadowski, Phys. Rev. Lett. 85, 2557 (2000)

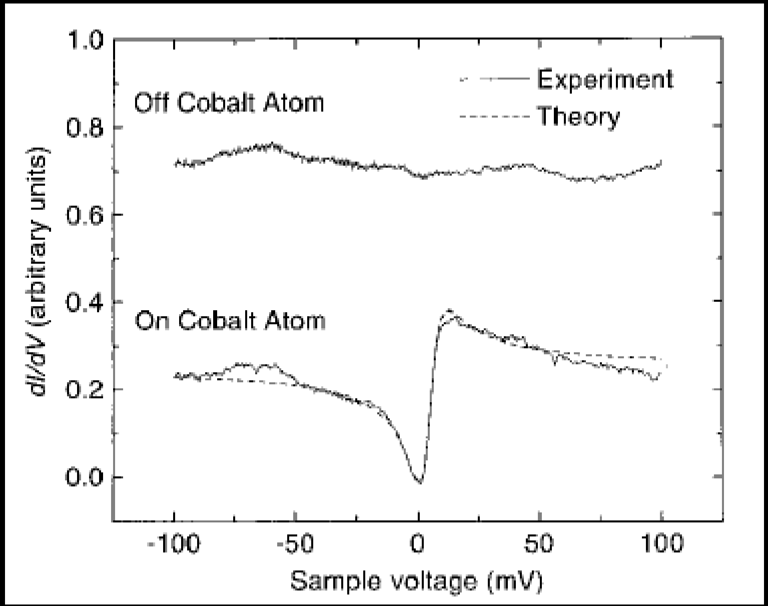
Single Magnetic Adatom Kondo Resonance



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

‘Fano Spectrum’ of Kondo Resonance

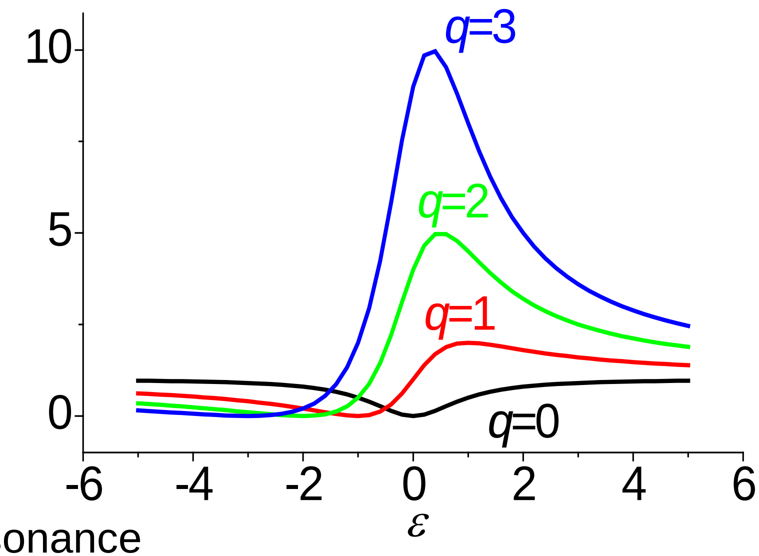




V. Madhavan *et al,* Science **280**, 567 (1998)
H. Manoharan *et al Nature* **403**, 512-515 (2000).
N. Knorr, *et al*. *Phys. Rev. Lett.* **88**, 096804 (2002).

Physical Significance of Fano Signature

$$g(r,E) \propto \frac{(q+E')^2}{E'^2+1};\; E' = \frac{(E-\varepsilon_0)}{\Gamma/2}$$



ε_0 energy of many-body state screening spin

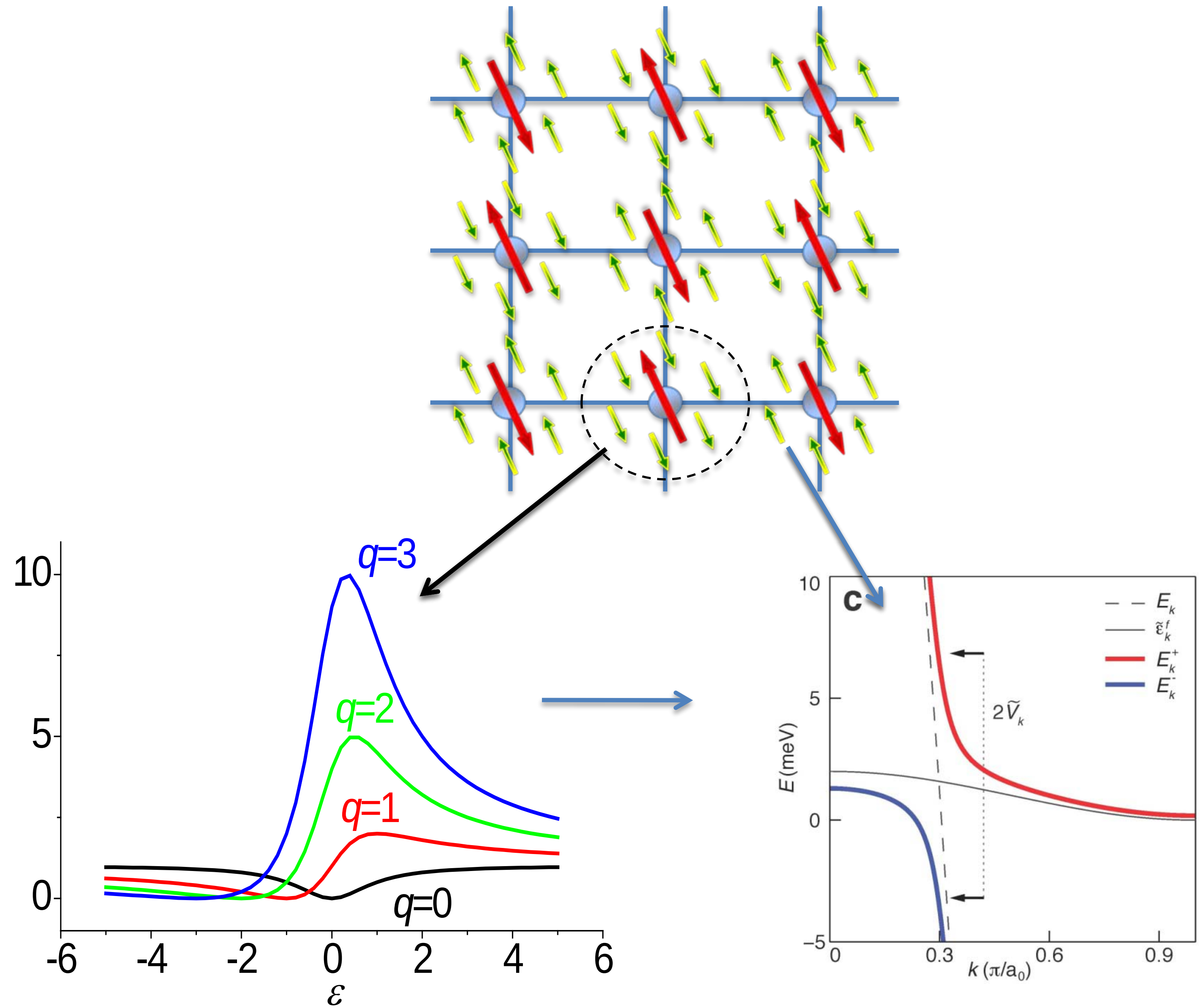
Γ width of resonance (simple Kondo $2k_BT_k$)

q Ratio of matrix elements linking tip state to resonance and to continuum

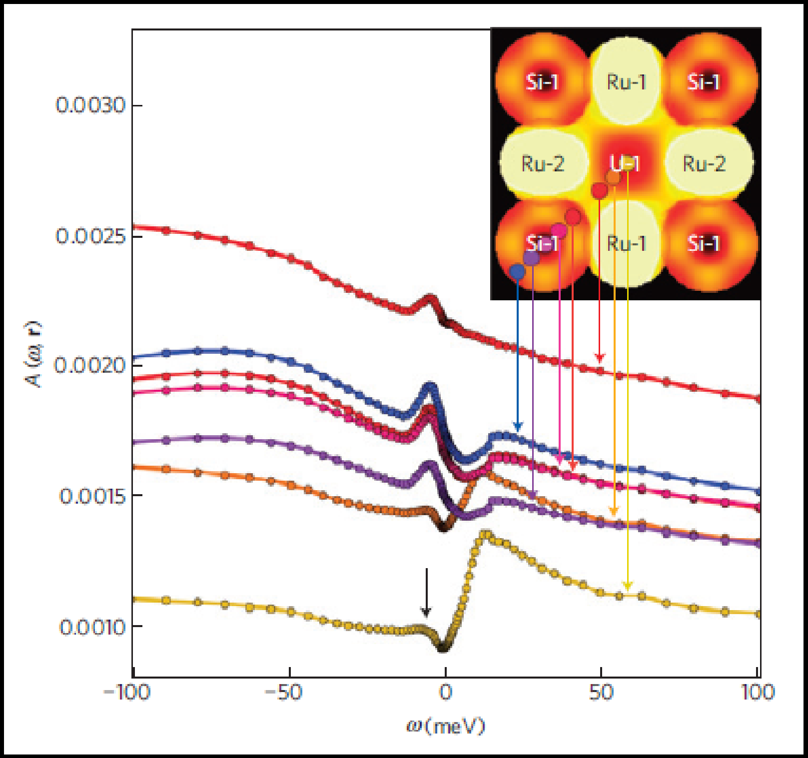
$$q(r) = \frac{\operatorname{Re} G(r) + t(r)}{\operatorname{Im} G(r)} \qquad t(r) = t_0 e^{-\frac{d(r)}{\alpha}}$$

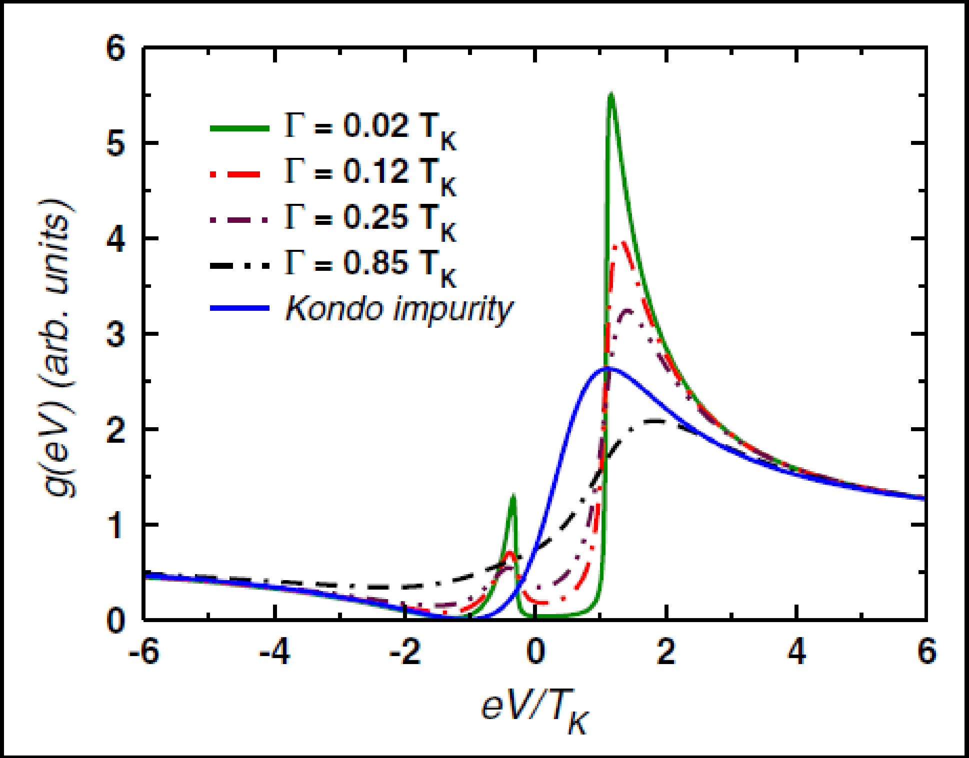
M. Plihal und J.W. Gadzuk, Phys. Rev. B 63, 085404 (2001)

Kondo Lattice system: Perhaps one might expect a 'Fano Lattice'?



'Fano Lattice' Theories





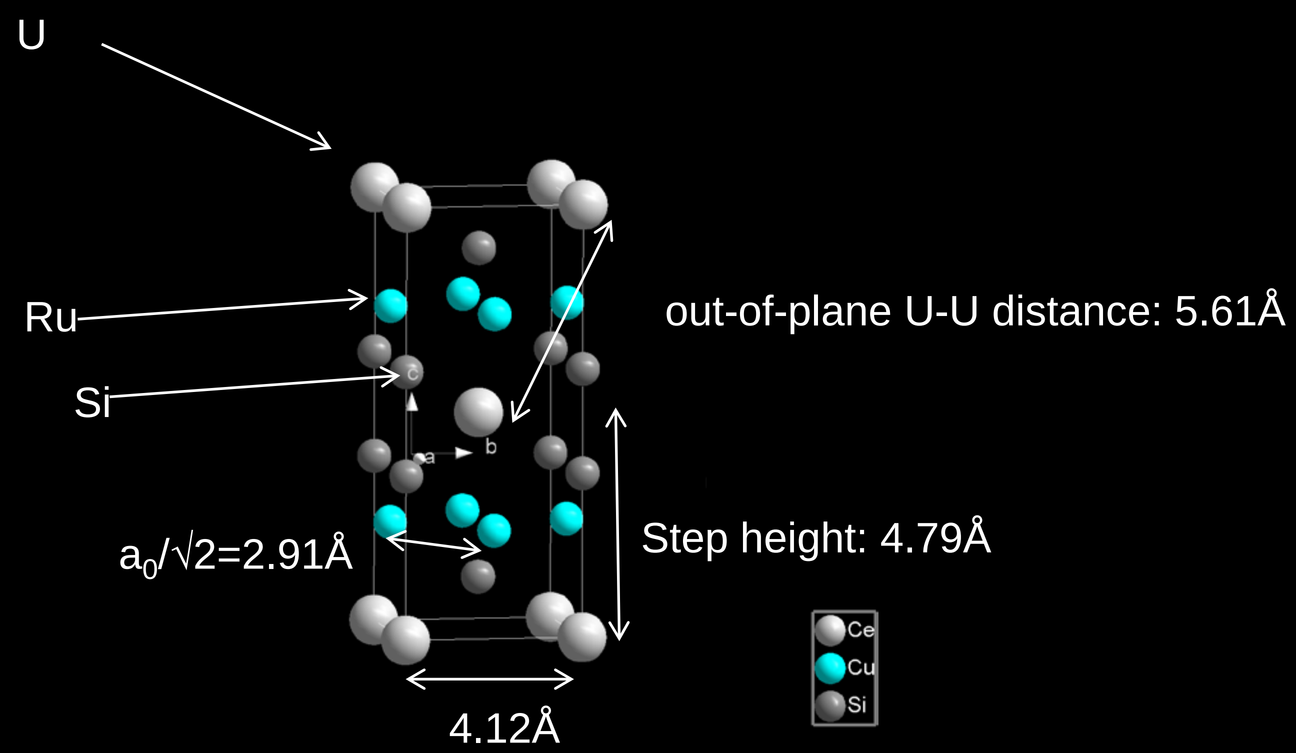
Haule K. & Kotliar G,
Nature Phys. **5**, 796 (2009).

Maltseva, M., Dzero, M. & Coleman P.
Phys. Rev. Lett. **10**, 206402 (2009)

URu_2Si_2

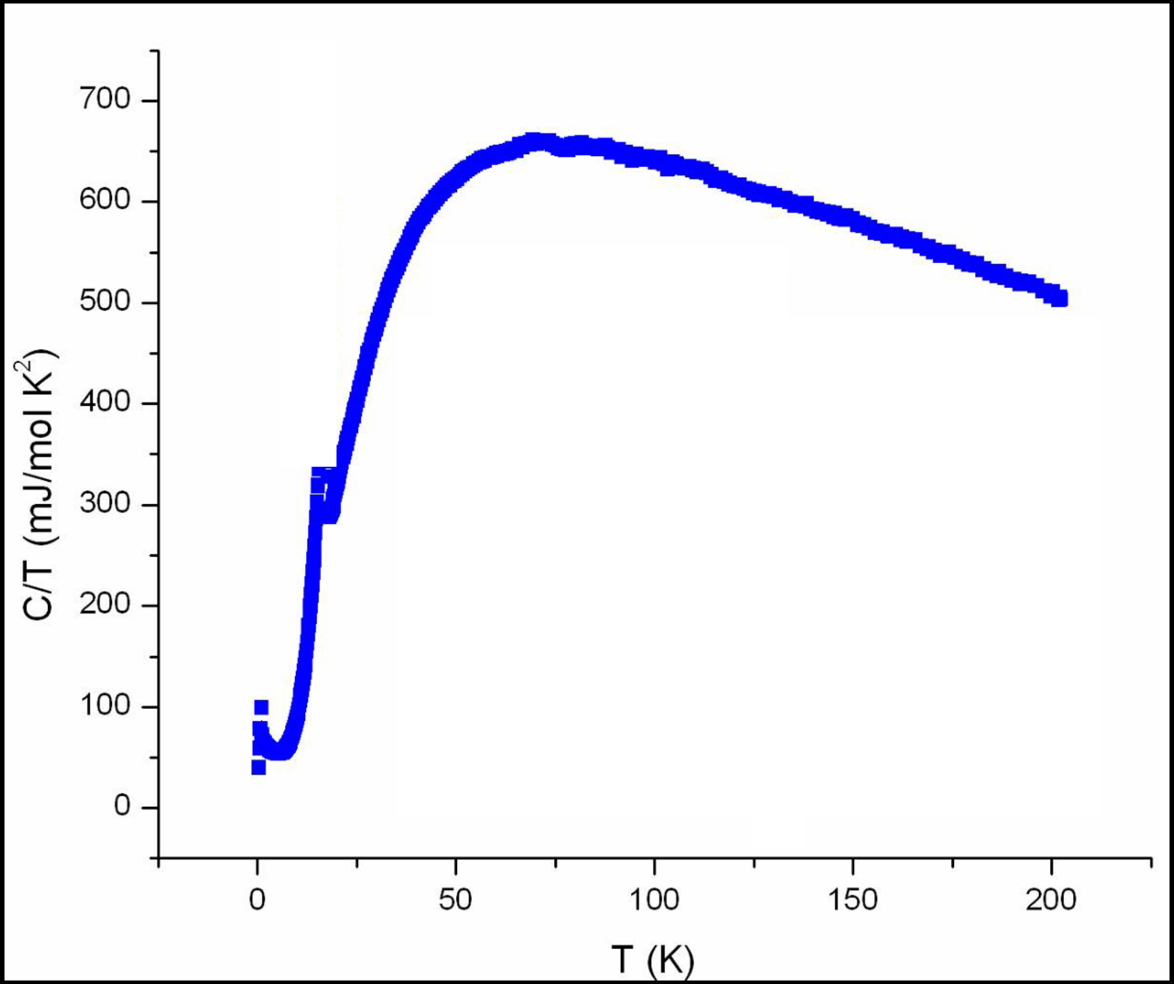
URu_2Si_2 is a modestly heavy fermion system

γ=100 mJ/mol K^2 m^*/m_e ~ 25

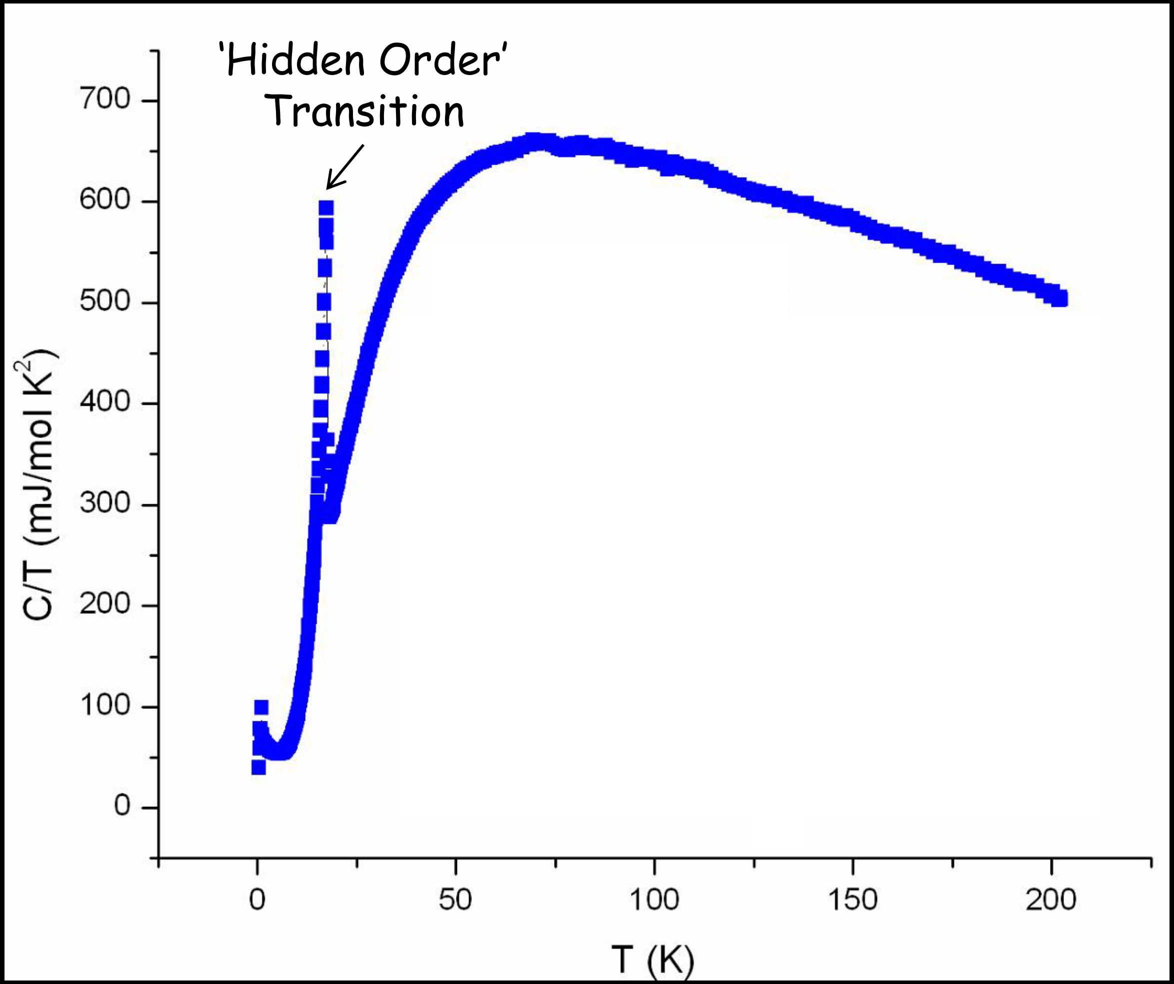


(same as $CeCu_2Si_2$ with U and Ru instead of Ce and Cu);
a=4.124Å; c=9.582Å (PRL65-3189)

URu_2Si_2 is a modestly heavy fermion system T*~55K

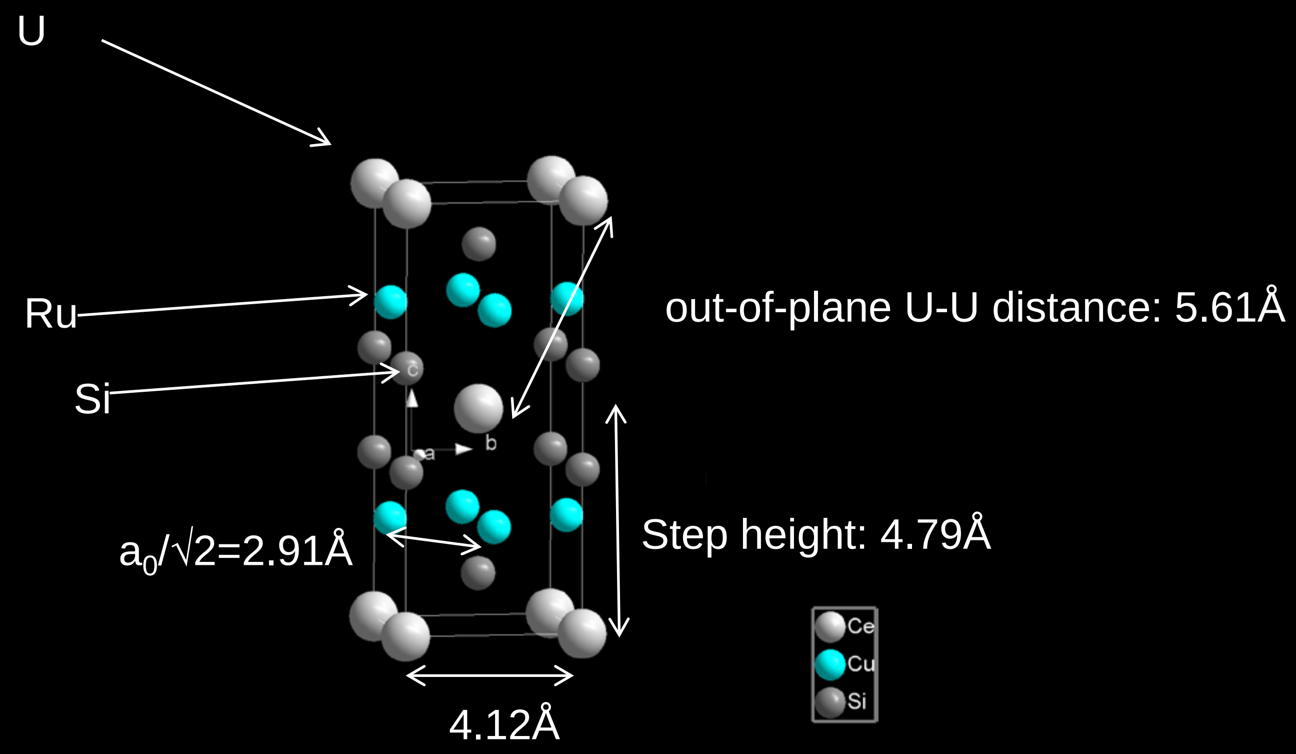


URu_2Si_2 is a modestly heavy fermion system T*~55K with an additional 'Hidden Order' phase transition at 17.5K



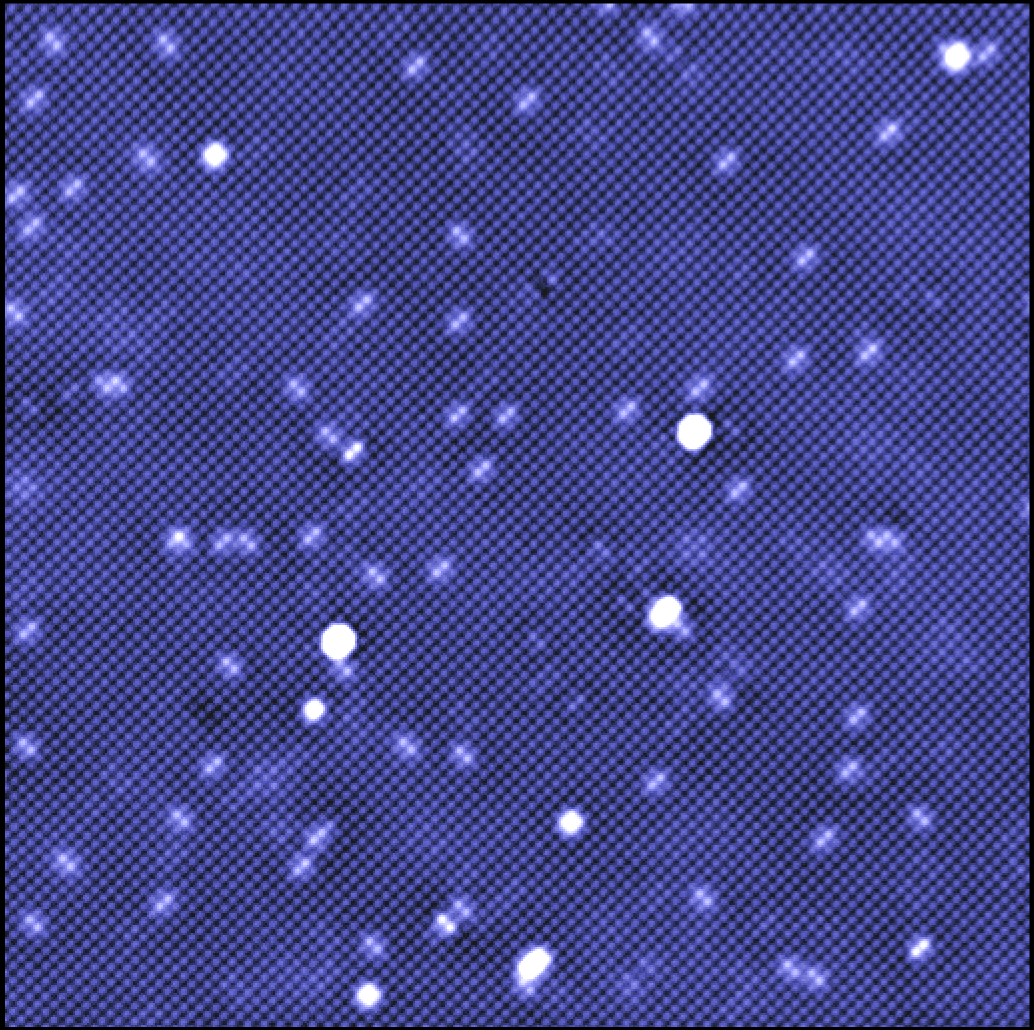
Why URu_2Si_2 ?

γ=100 mJ/mol K^2 m^*/m_e ~ 25



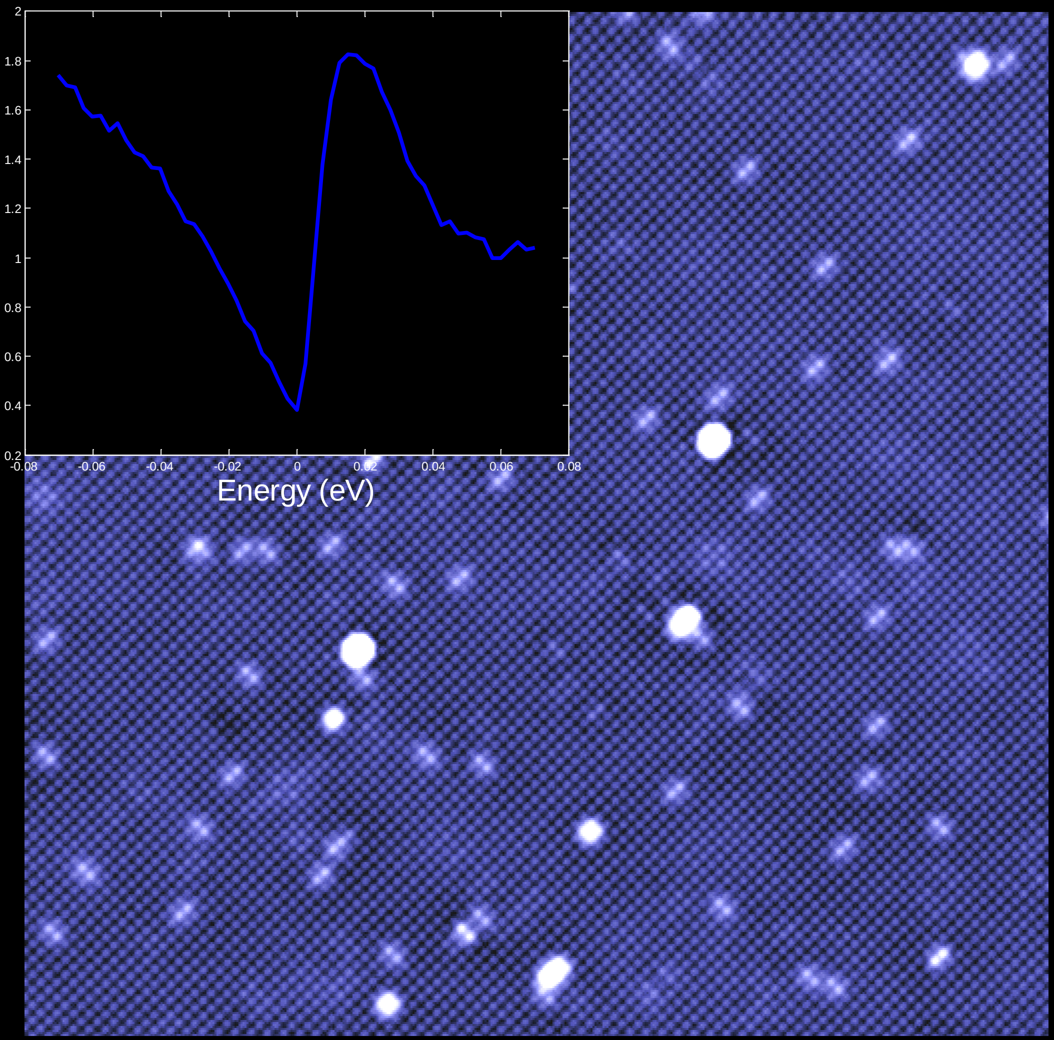
- Heavy fermion system
- Perfect cleave surface
- Lattice of f-atoms at surface
- Scattering interference

Si-layer termination



40nm x 40nm Si surface topography
(70619)

Fano-like spectrum at every Si atom

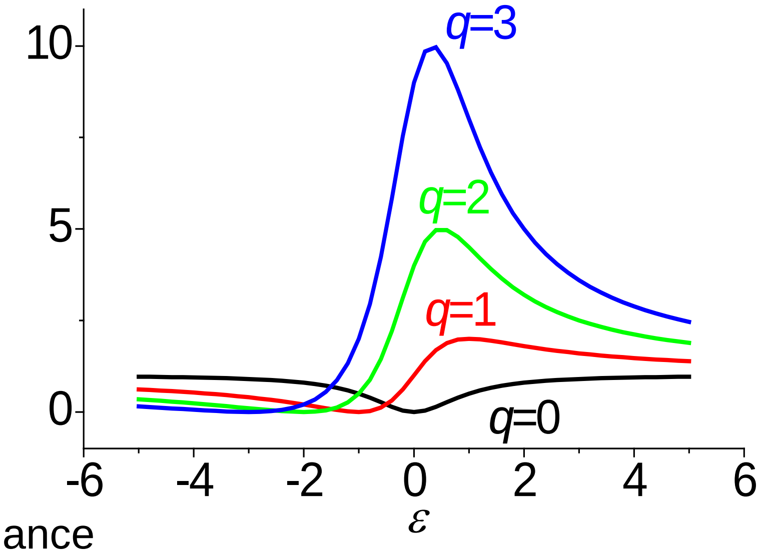


40nm x 40nm topography

A.R. Schmidt *et al* (2009)

Fano Signature Analysis

$$g(r,E) \propto \frac{(q+E')^2}{E'^2+1};\ E' = \frac{(E-\varepsilon_0)}{\Gamma/2}$$



ε_0 energy of many-body state screening spin

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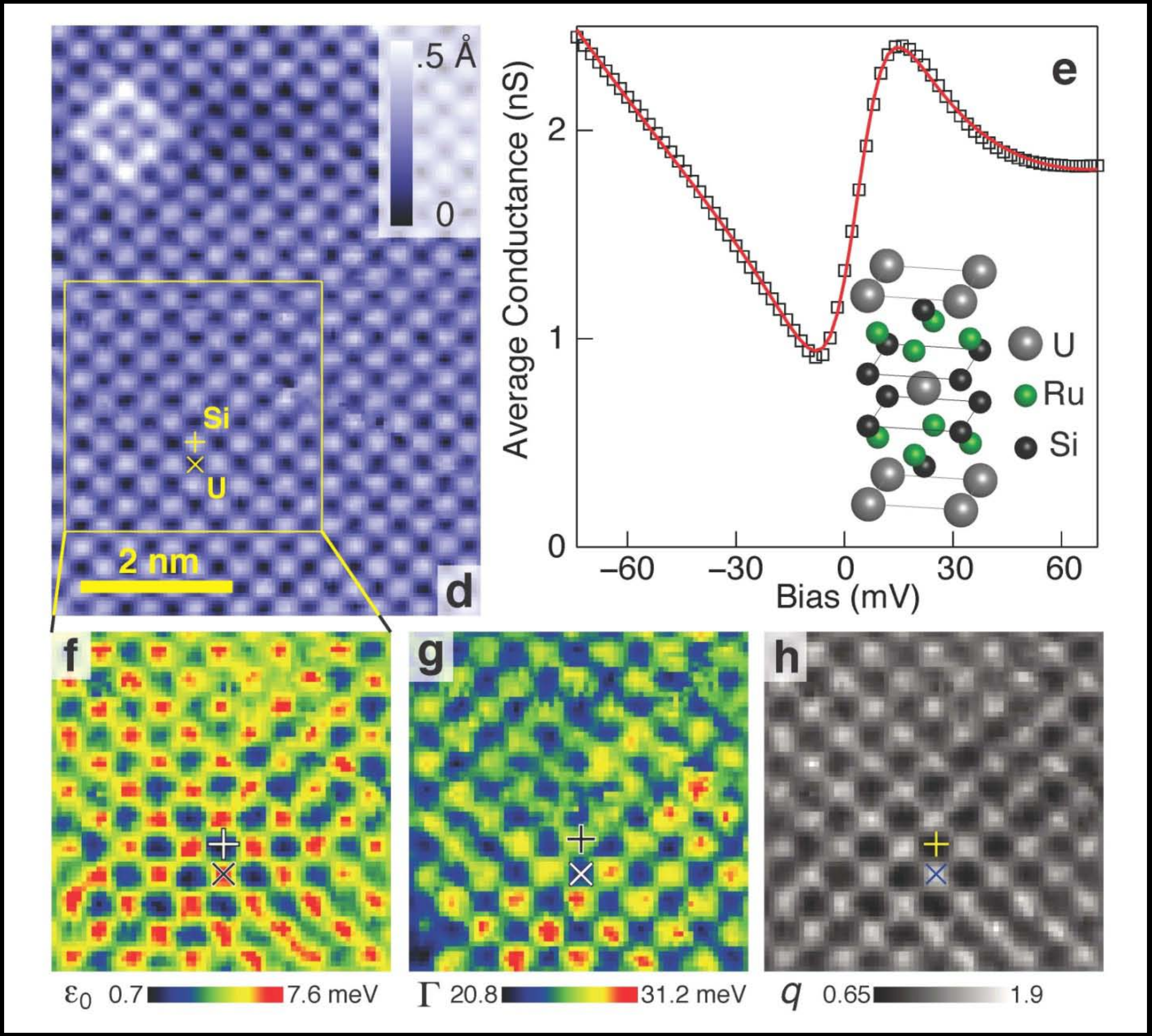
M. Plihal und J.W. Gadzuk, Phys. Rev. B 63, 085404 (2001)

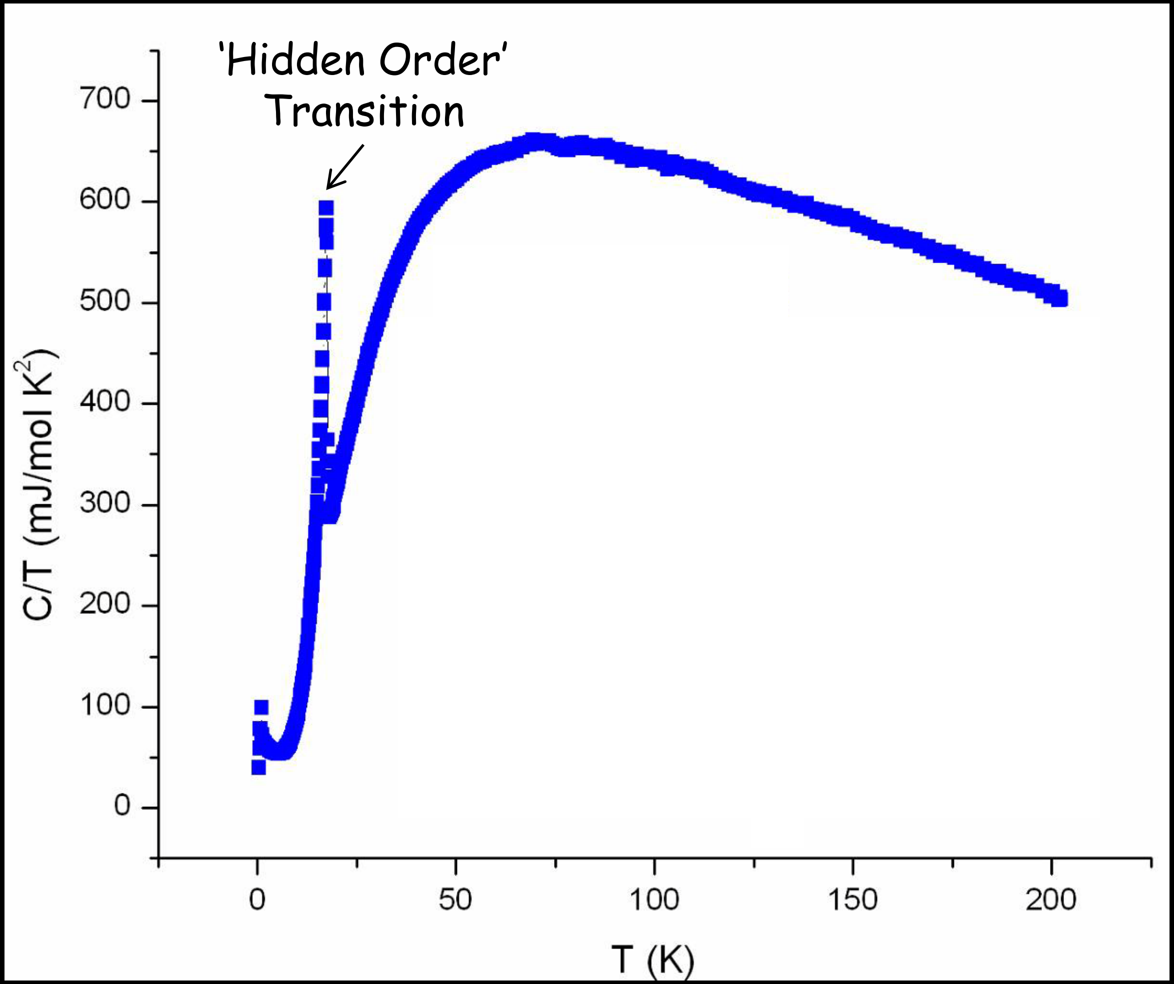
'Fano Lattice' Electronic Structure $(T>T_O)$



A.R. Schmidt *et al* (2009)

URu_2Si_2 'Hidden Order' State

'Hidden Order' Transition T_o=17.5K



'Hidden Order' Transition T_o=17.5K

- Heavy fermion material
- Superconductor below T_c~1.5K
- Energy-gap ~10+-2 mV (Photo, INS, Cp)

• Palstra, T.T.M., Menovsky, A.A., & Mydosh, J.A. Superconducting and magnetic transitions in the heavy-fermion system URu_2Si_2. *Phys. Rev. Lett.* **55**, 2727-2730 (1985).

•[Broholm, C. *et al*. Magnetic excitations and order in the heavy-electron superconductor URu_2Si_2. *Phys. Rev. Lett.* **58**, 1467-1470 (1987).

• Bonn, D.A. *et al.* Far-infrared properties of URu_2Si_2. *Phys. Rev. Lett.* **61**, 1305-1308 (1988).

• Wiebe, C.R. *et al*. Gapped Itinerant spin excitations account for missing entropy in the hidden order state of URu_2Si_2. *Nature Phys.* **3**, 96-99 (2007).

•] Santander-Syro, A.F. *et al.* Fermi-surface instability at the 'hidden-order' transition of URu_2Si_2. *Nature Phys.* **5**, 637-641 (2009).

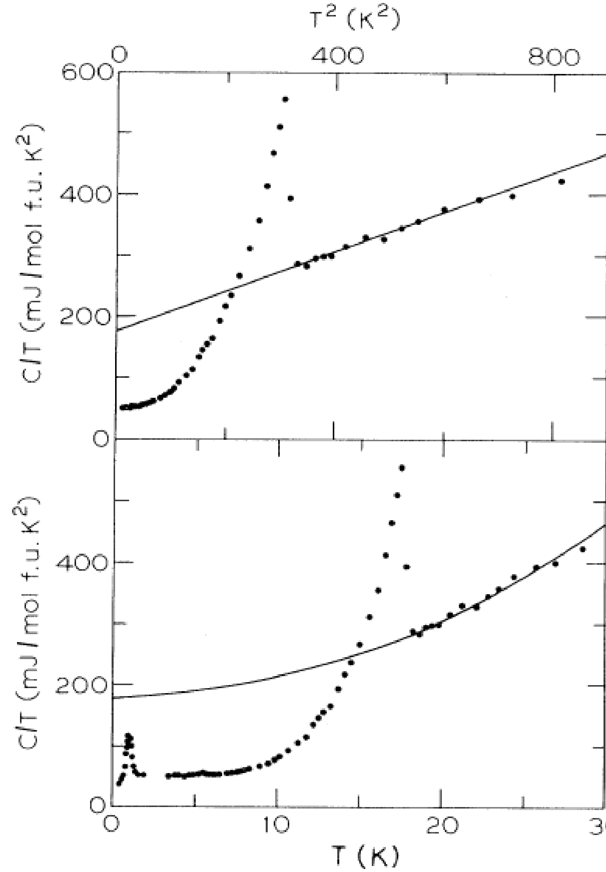


FIG. 1. Specific heat of URu_2Si_2 plotted as C/T vs T^2 (above) yielding γ and Θ_D, and as C/T vs T (below) showing the entropy balance.

‘Hidden Order’ Transition T_o=17.5K

‘Conventional’ Density Wave

Broholm, C. *et al.* Magnetic excitations in the heavy-fermion superconductor URu_2Si_2. *Phys. Rev. B.* **43**, 809-822 (1991).

Ikeda, H. & Ohashi, Y. Theory of unconventional spin density wave: a possible mechanism U-based heavy fermion compounds. *Phys. Rev. Lett.* **81**, 3723-3726 (1998).

Chandra, P. *et al.* Hidden orbital order in the heavy fermion metal URu_2Si_2. *Nature* **417**, 831-834 (2002).

Varma, C.M. & Lijun, Z. Helicity order: Hidden order parameter in URu_2Si_2. *Phys. Rev. Lett*. **96**, 036405-1-036405-4 (2006).

Balatsky, A.V. *et al.* Incommensurate spin resonance in URu_2Si_2. *Phys. Rev. B*. **79**, 214413 (2009).

‘Altered’ Kondo Effect

Santini, P. Crystal field model of the mag properties of URu_2Si_2. *Phys. Rev. Lett.* **73**, 1027-1030 (1994).

Barzykin, V. & Gor’kov, L.P. Singlet magnetism in heavy fermions. *Phys. Rev. Lett.* **74**, 4301-4304 (1995).

Haule K. & Kotliar G. Arrested Kondo effect and hidden order in URu_2Si_2. *Nature Phys.* **5**, 796-799 (2009).

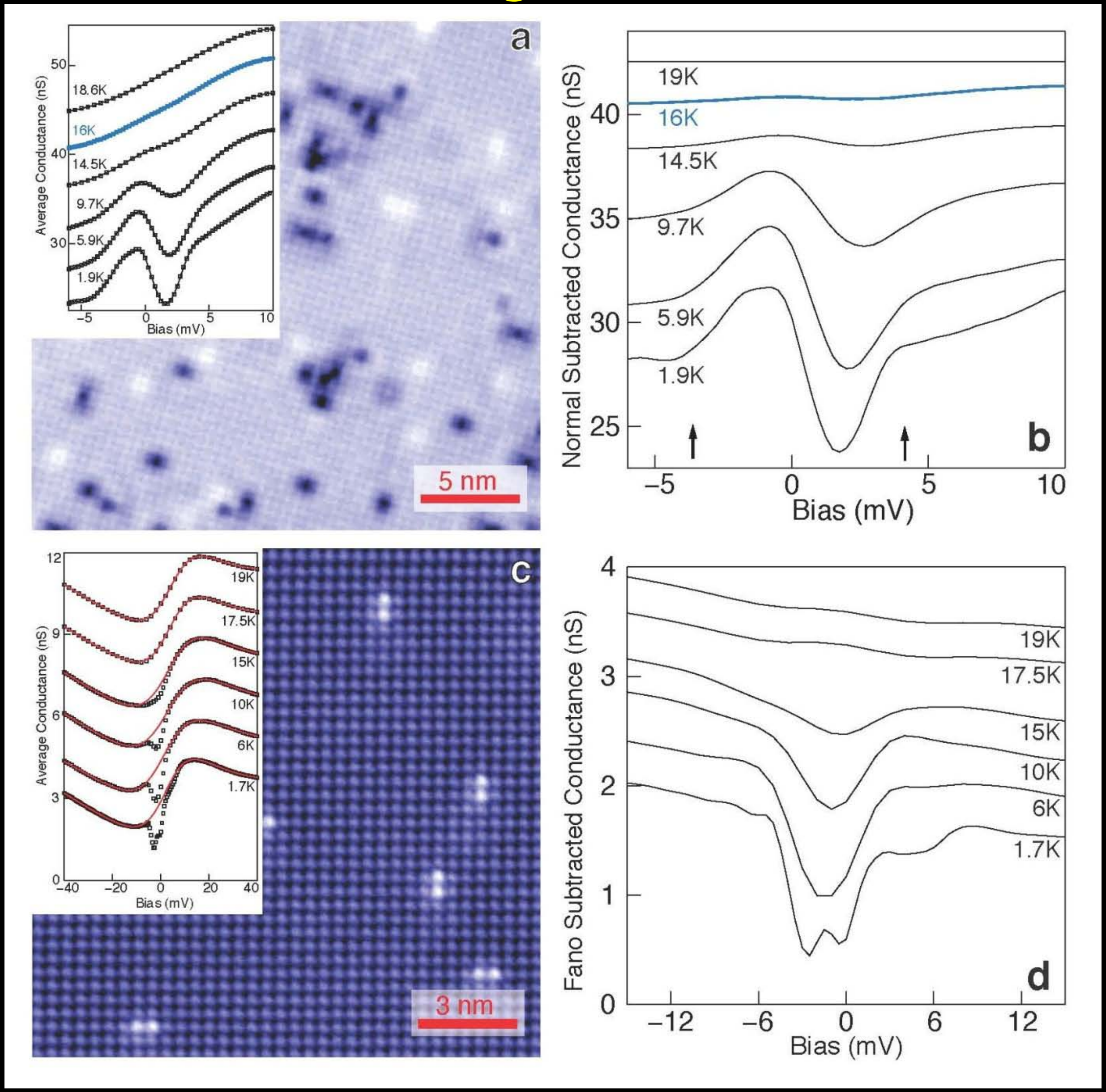
Haule K. & Kotliar G. Complex Landau Ginzburg theory of the hidden order of URu_2Si_2. Preprint available arXiv:0907.3892.

Emergence of 'Hidden Order' DOS(E) from the Heavy Fermion Fano Spectrum

Alterations in Fano signature at HO Transition

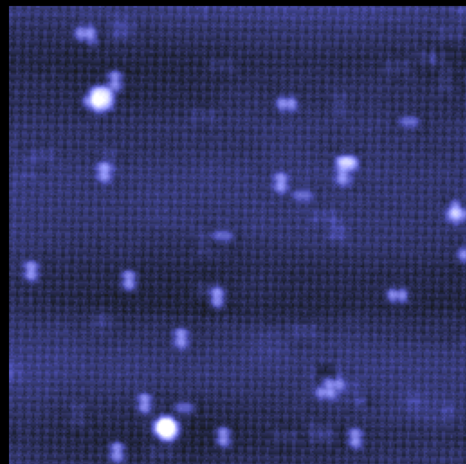
U-terminated

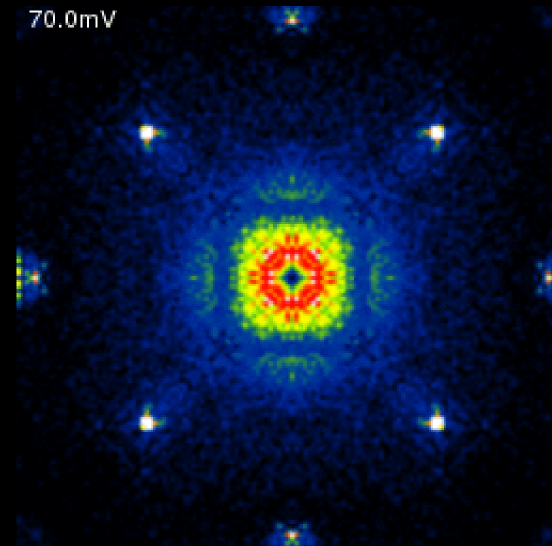
Si-terminated



A.R. Schmidt *et al* (2009)

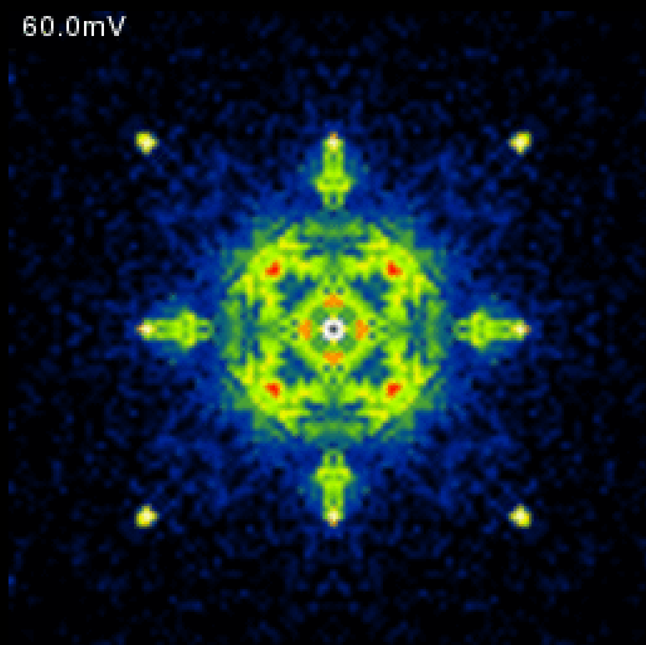
Si-layer Quasiparticle Interference Imaging

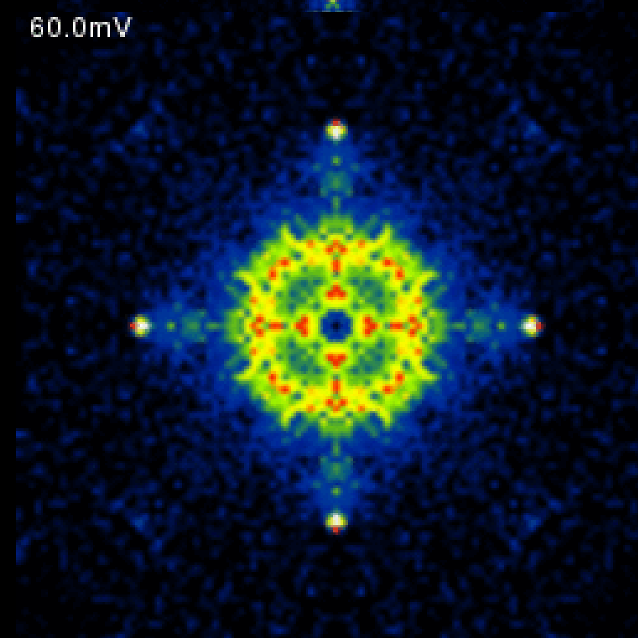




4

12

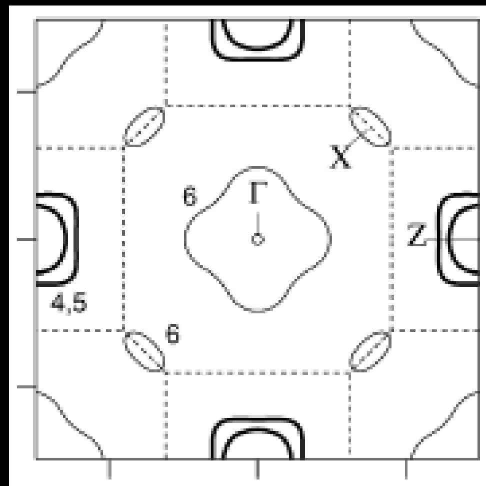


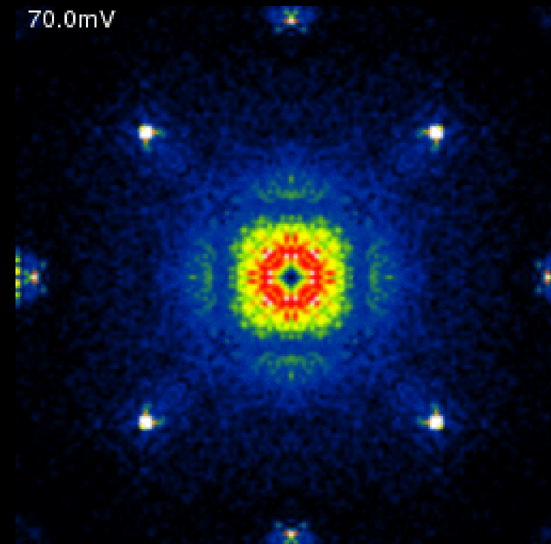


20

Rotated to overlap with 4.2K map

QPI inversion to identify bands was unachievable





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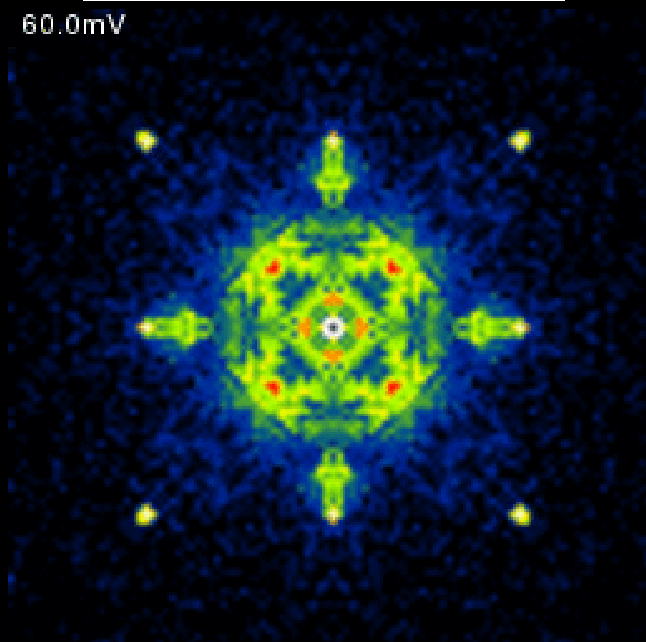
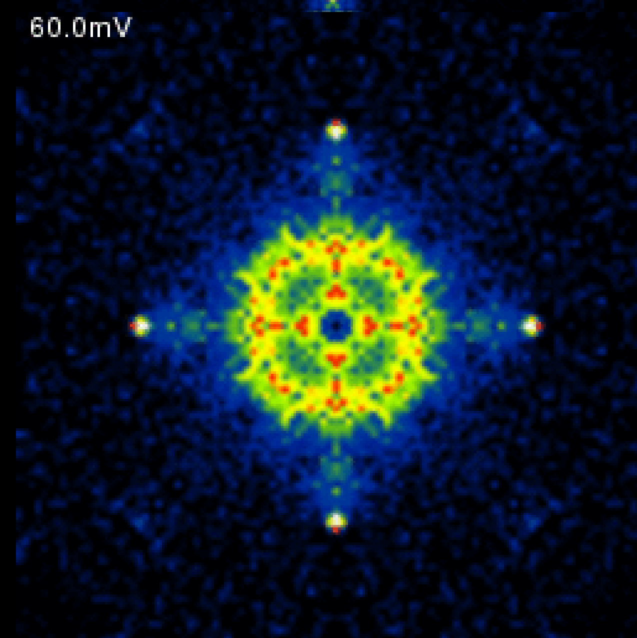
12



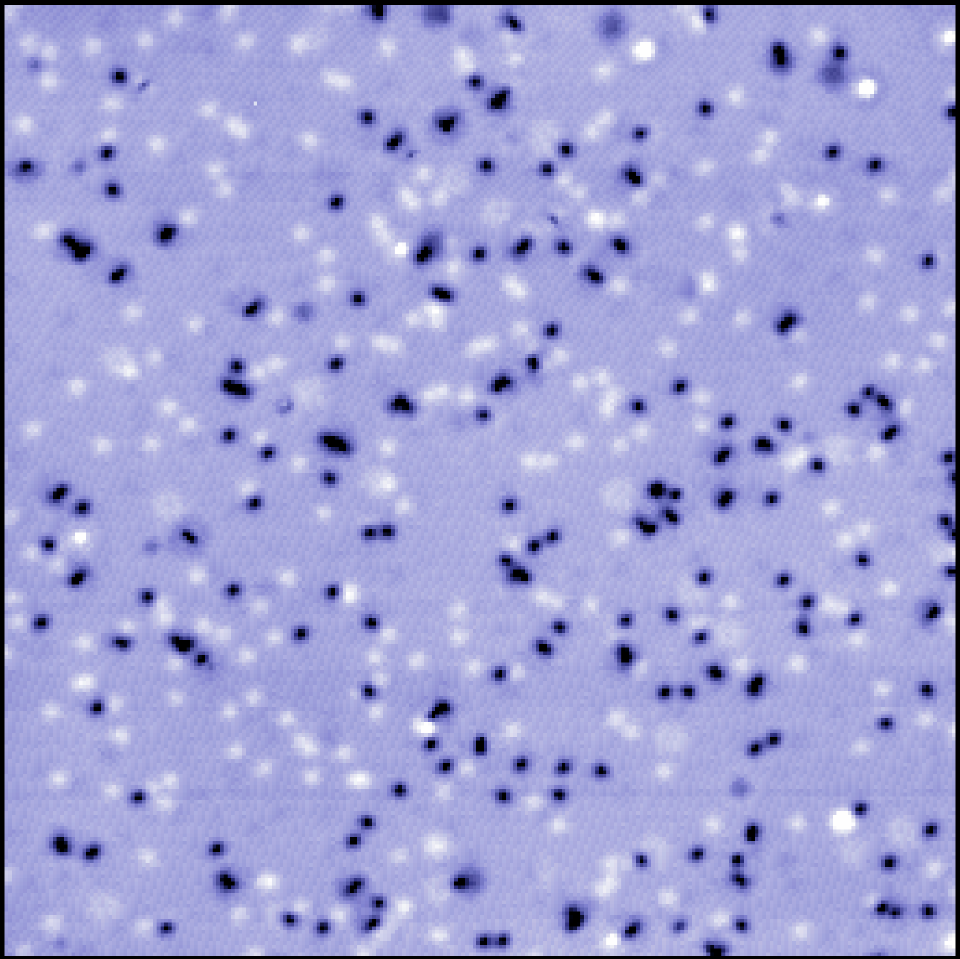


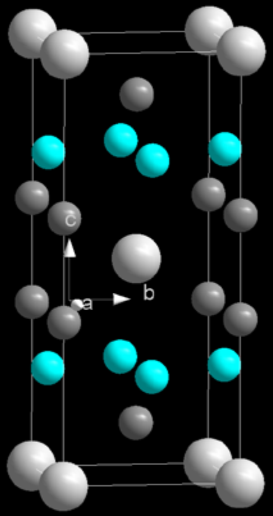
20

Rotated to overlap with 4.2K map

U-layer termination

$U_{0.99}Th_{0.01}Ru_2Si_2$

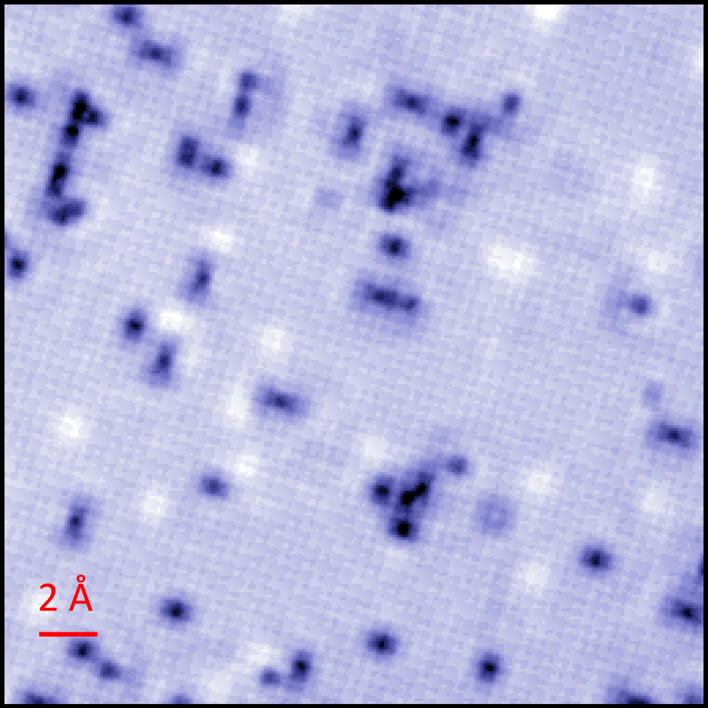


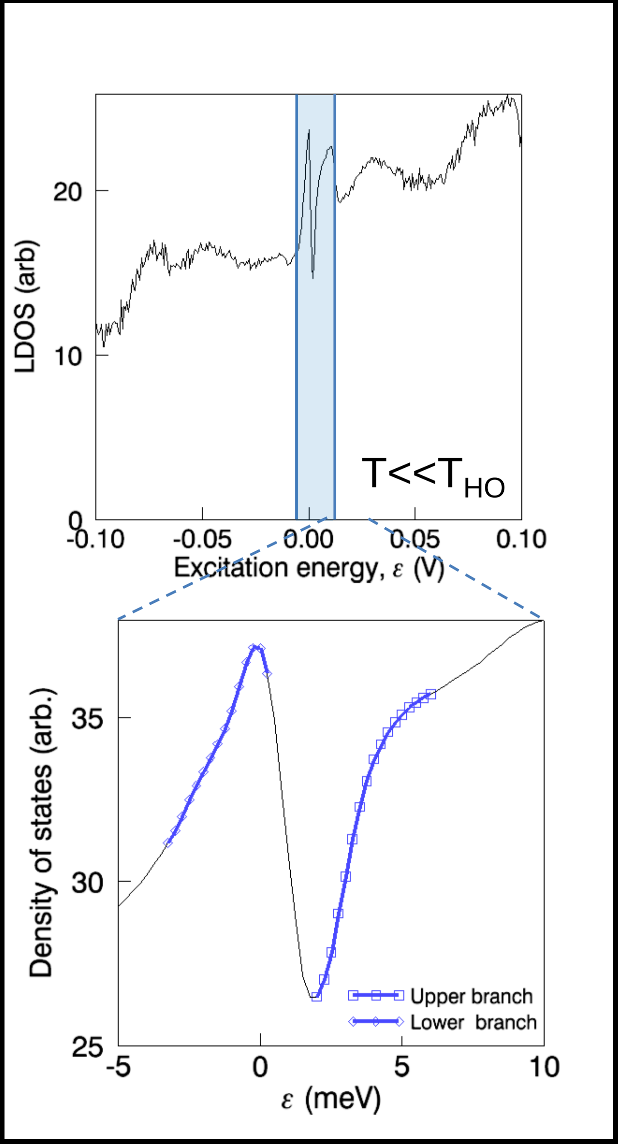


40nm x 40nm Topography
(70619)

A.R. Schmidt *et al* (2009)

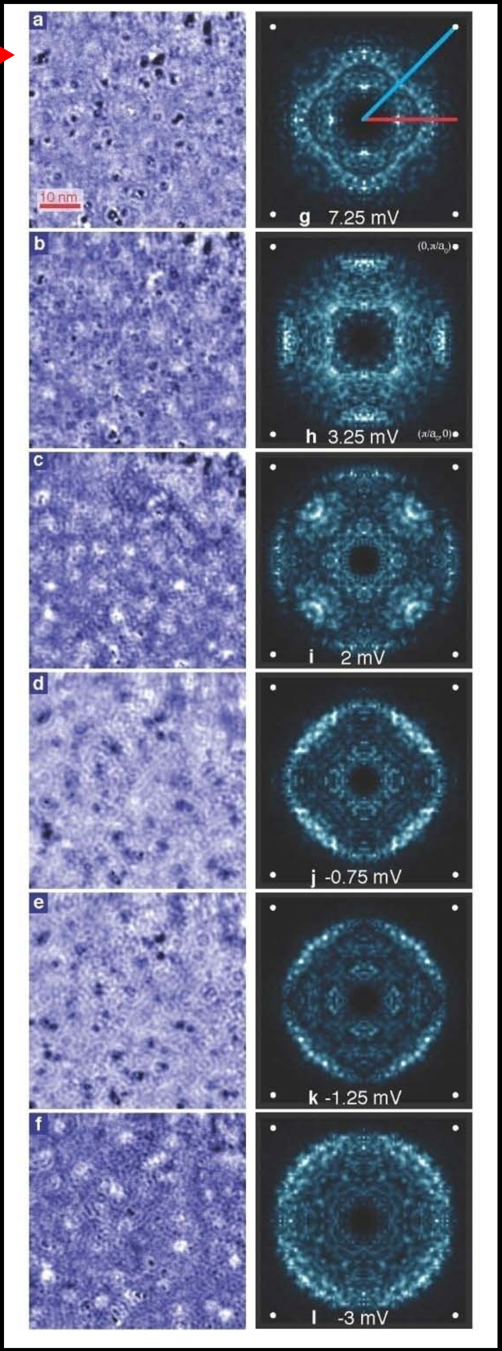
Signature of HO near E=0 on dI/dV spectrum at U-layer





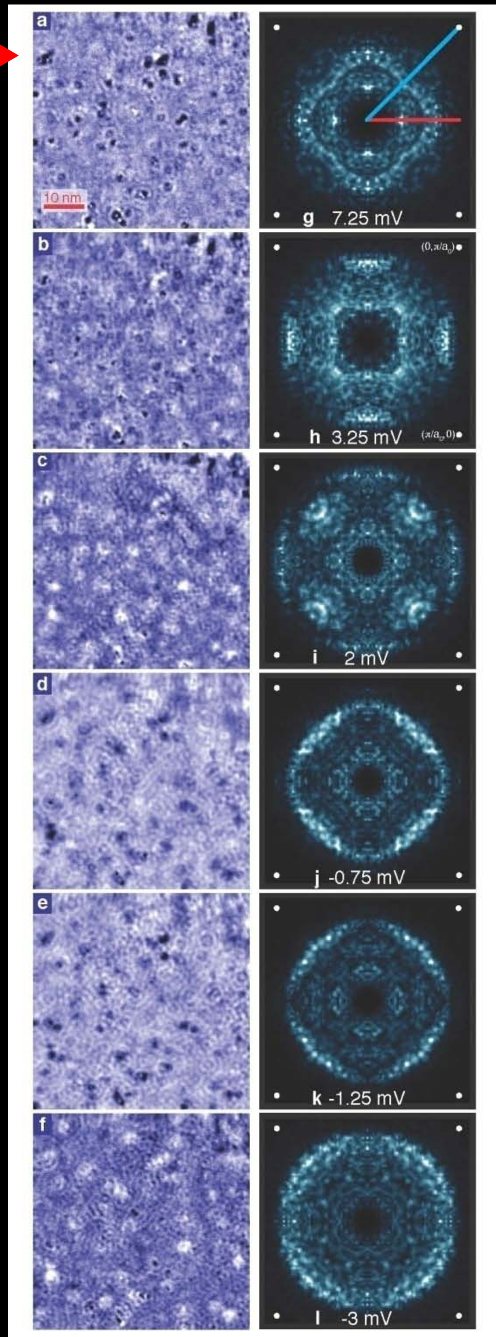
A.R. Schmidt *et al* (2009)

T=1.9K



A.R. Schmidt *et al* (2009)

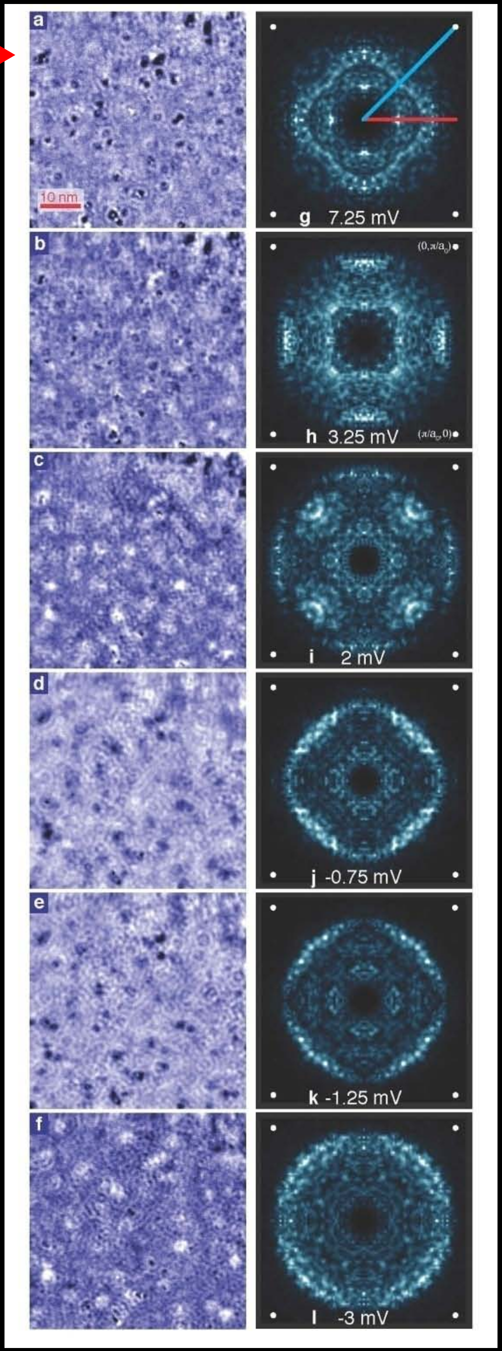
T=1.9K



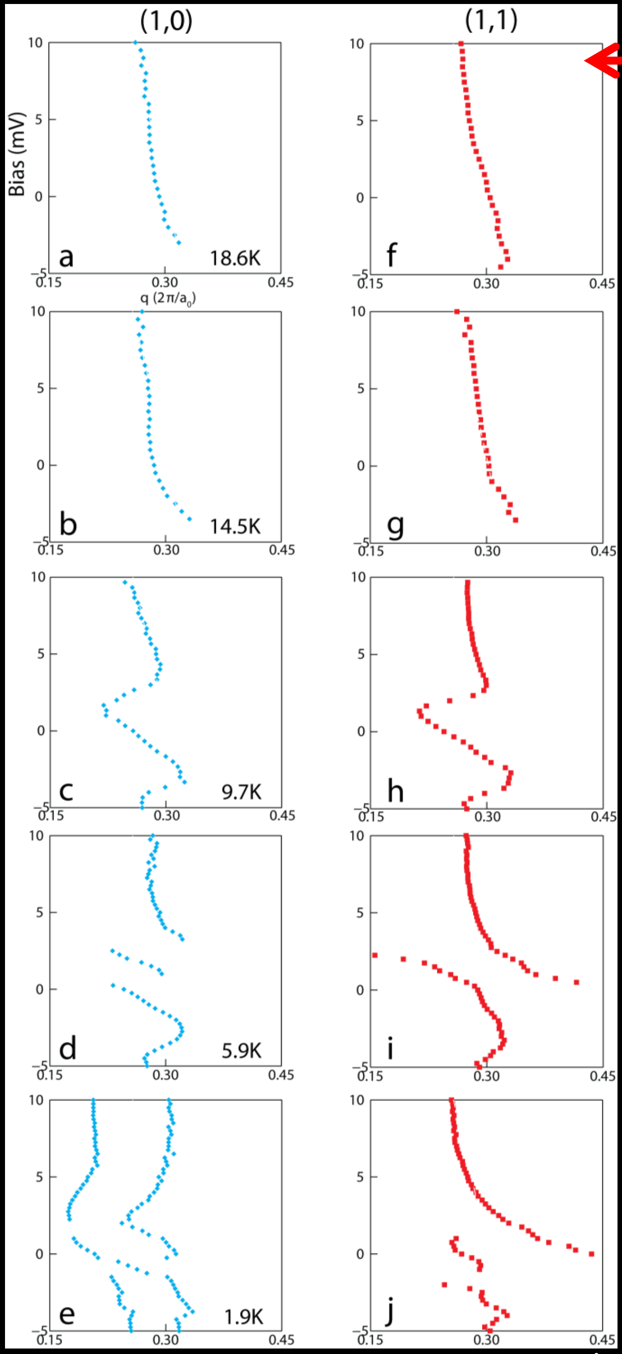
- Extremely rapid k(E) – heavy fermions
- Within range of hidden-order gap only
- Highly anisotropic QPI & gap structure
- Completely different E<0 : E>0
- No static Q* (density wave) at any energy

A.R. Schmidt *et al* (2009)

T=1.9K



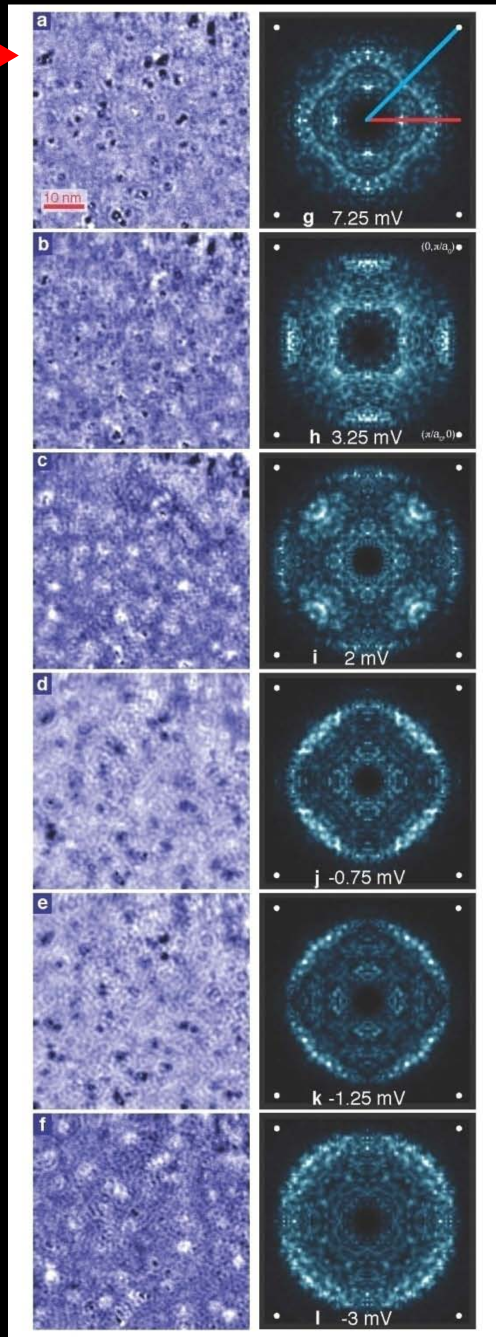
T dependence

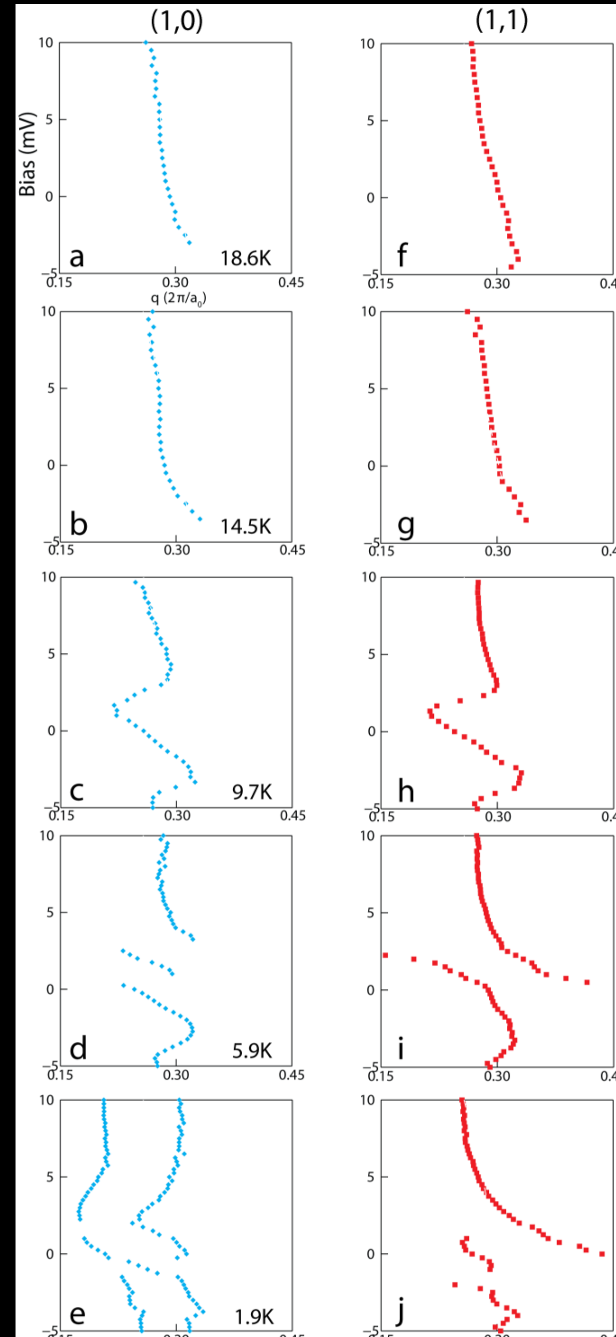


q

A.R. Schmidt *et al* (2009)

T=1.9K



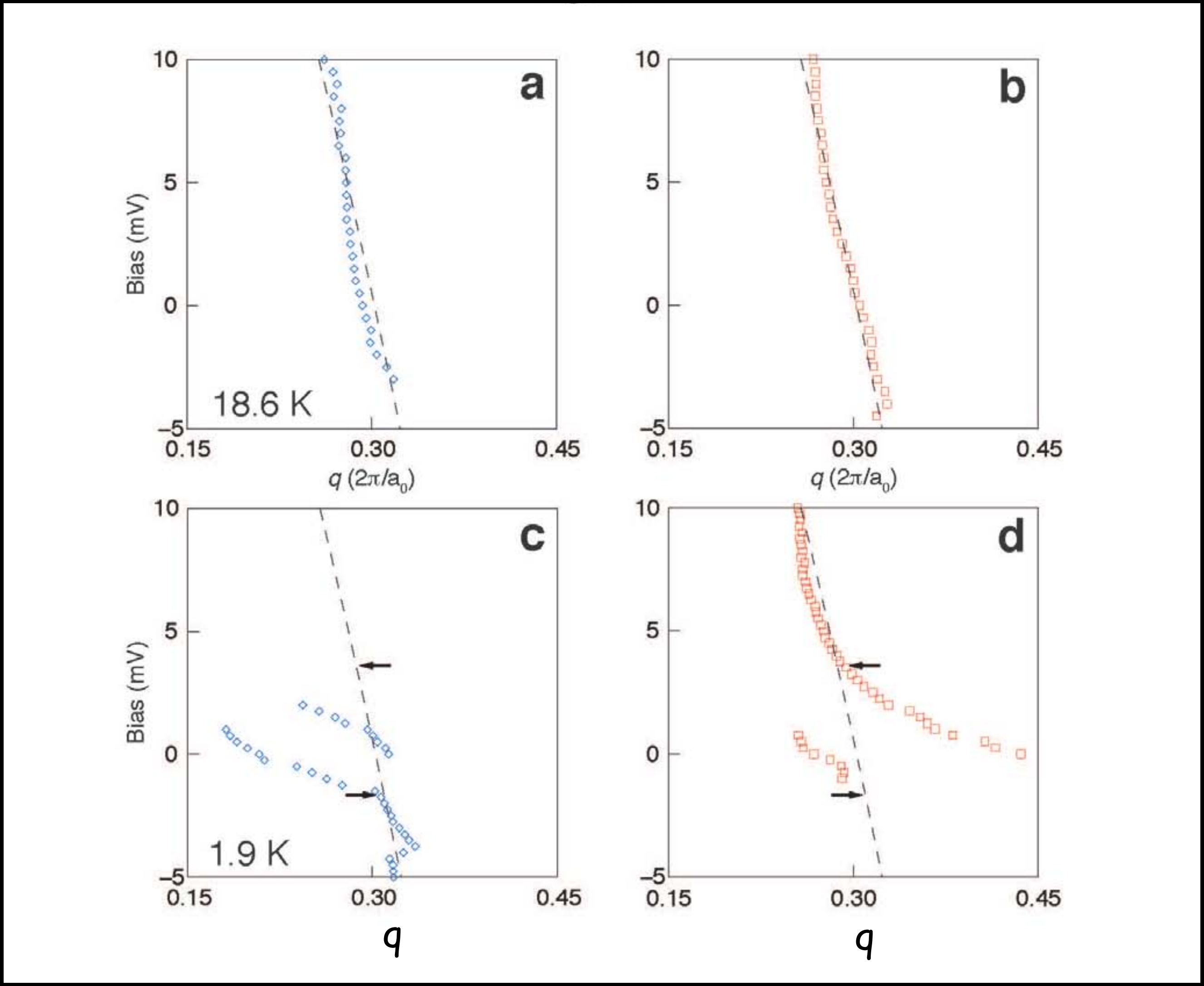


Extremely rapid T-dependence of band structure

q

A.R. Schmidt *et al* (2009)

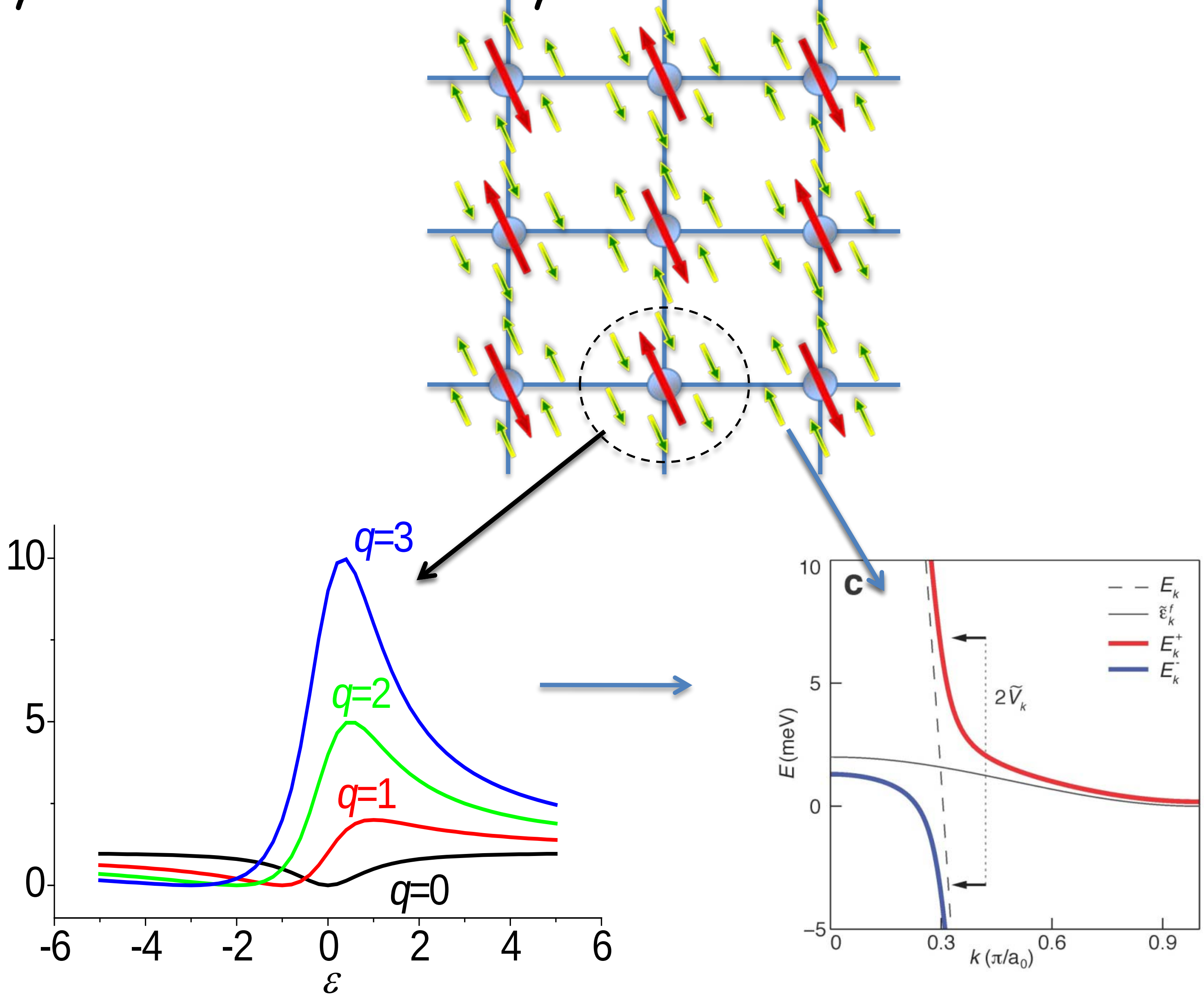
‘Hidden Order’ splits light band into two heavy bands



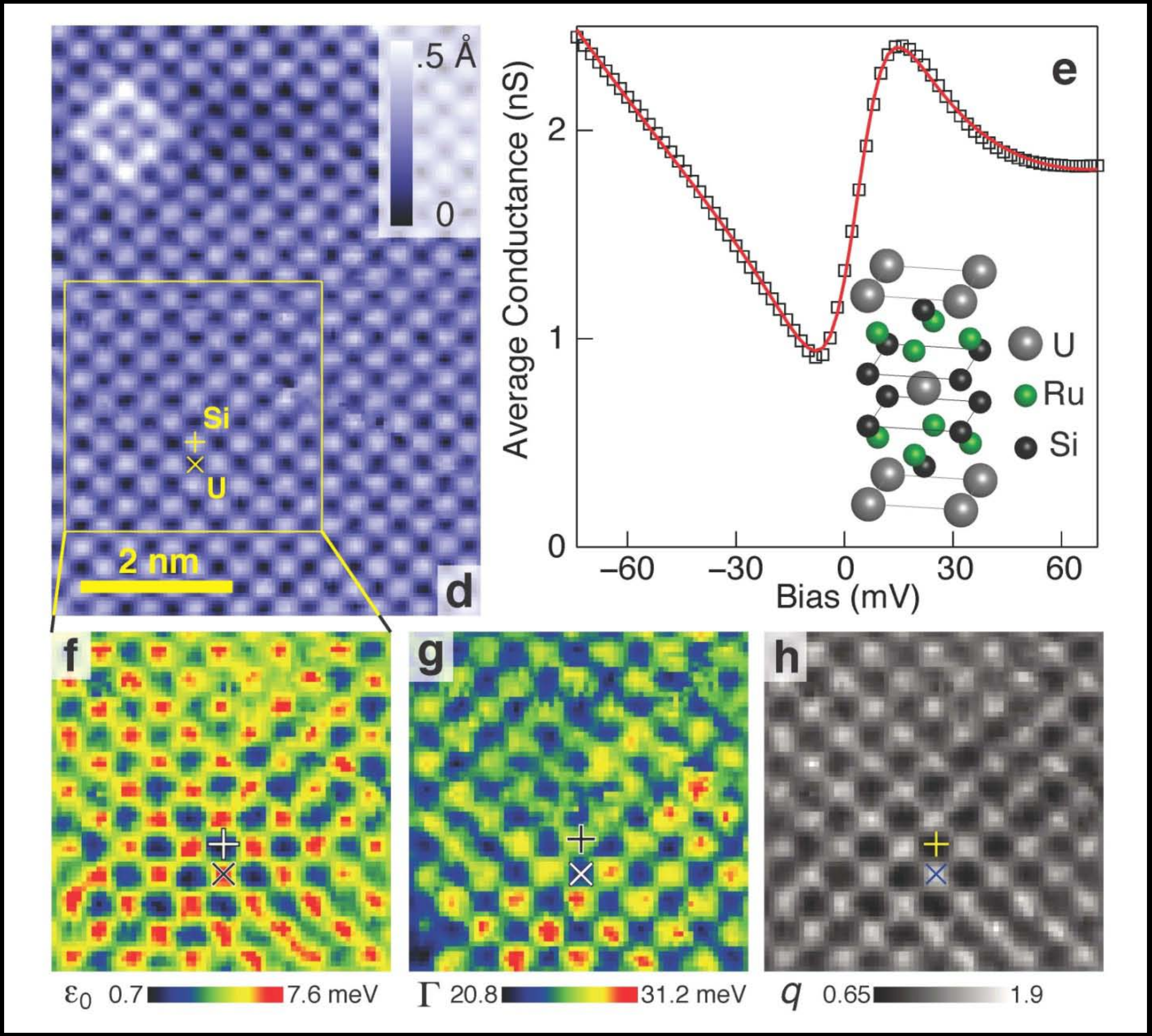
A.R. Schmidt *et al* (2009)

Conclusions

Challenge: atomically resolved image of d-f electron hybridization and heavy band formation in Kondo lattice?



'Fano Lattice' Imaging: New approach to heavy fermion physics



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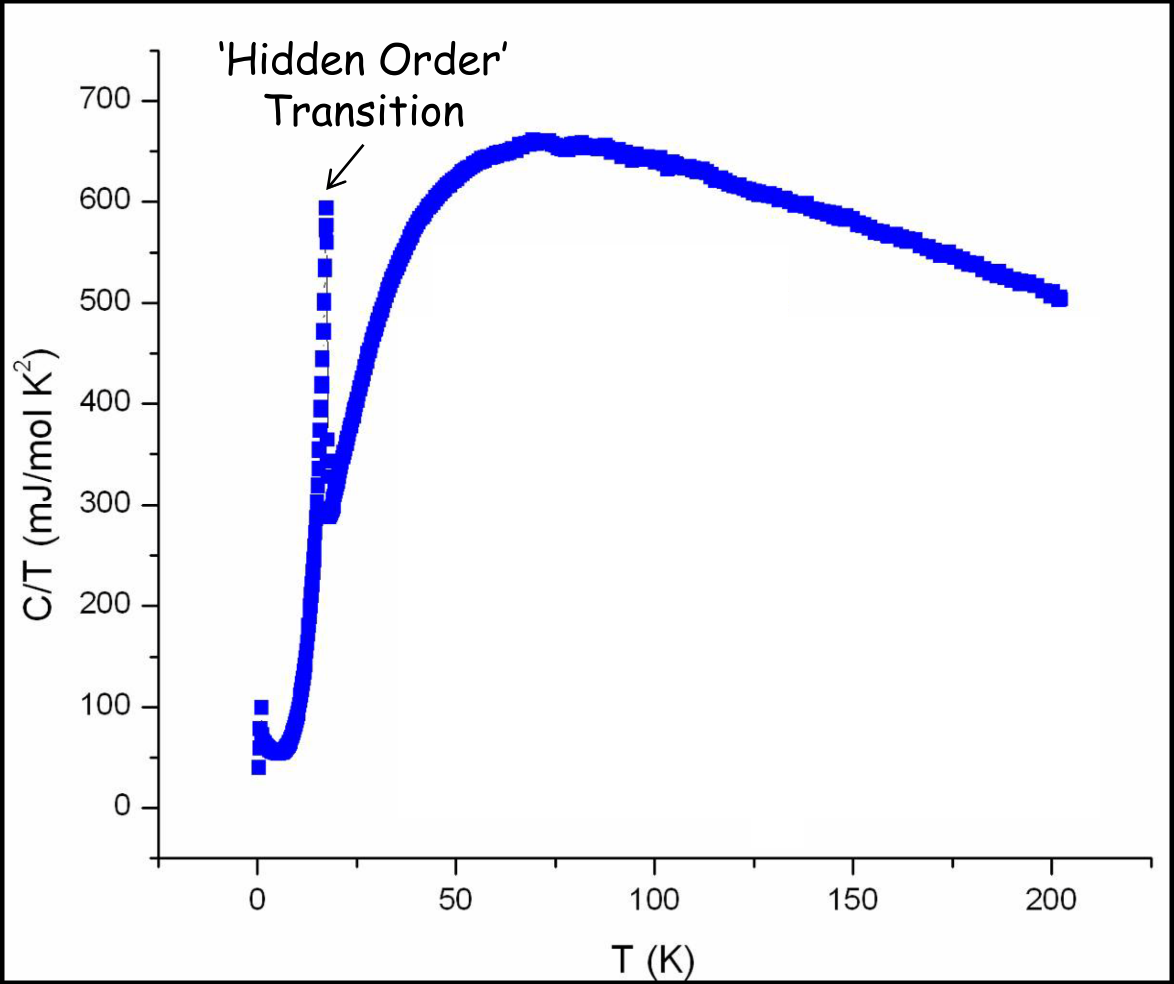
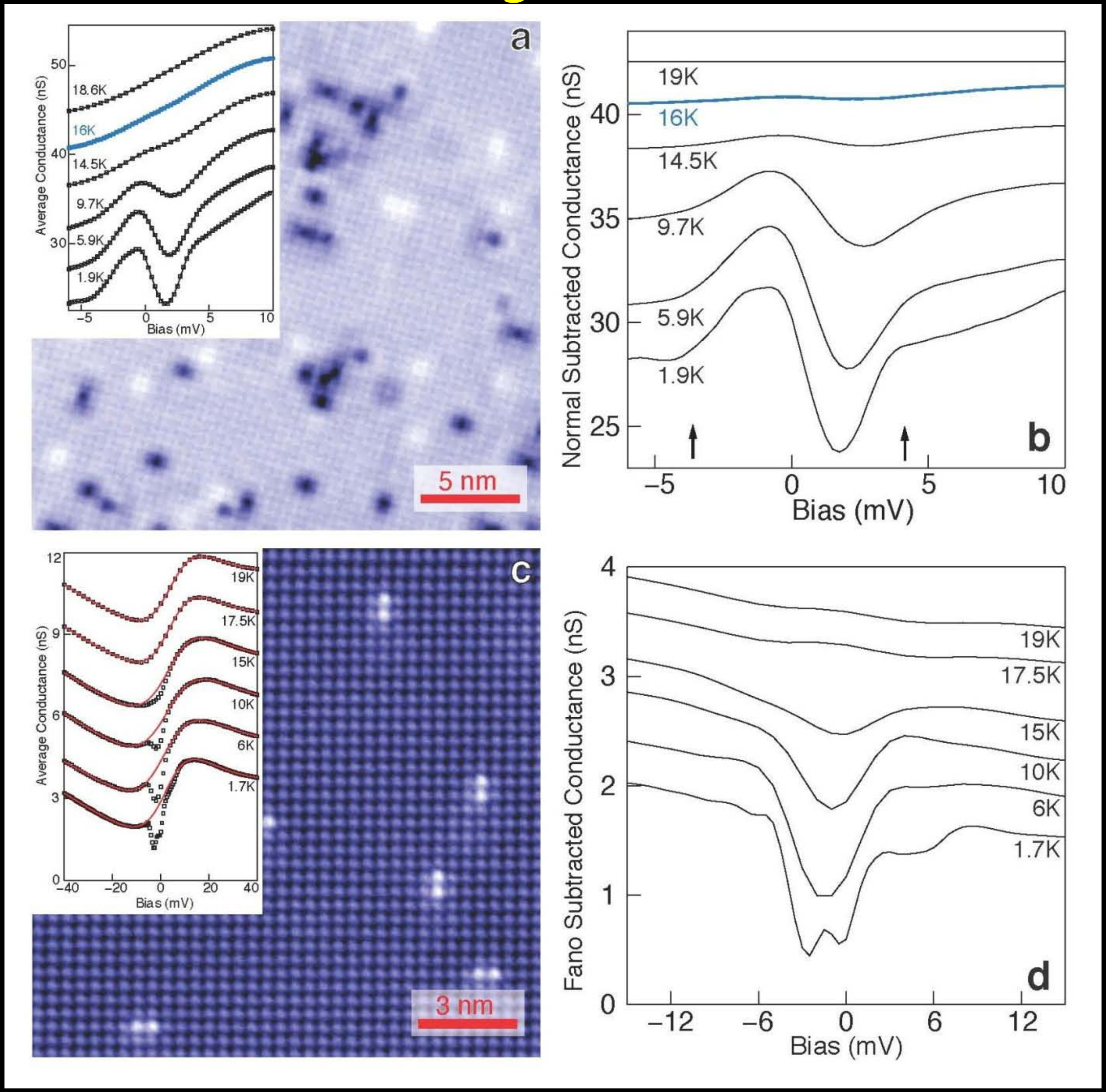
'Hidden Order' Transition T_o=17.5K



HO transition in LDOS emerges from 'Fano Lattice' signature



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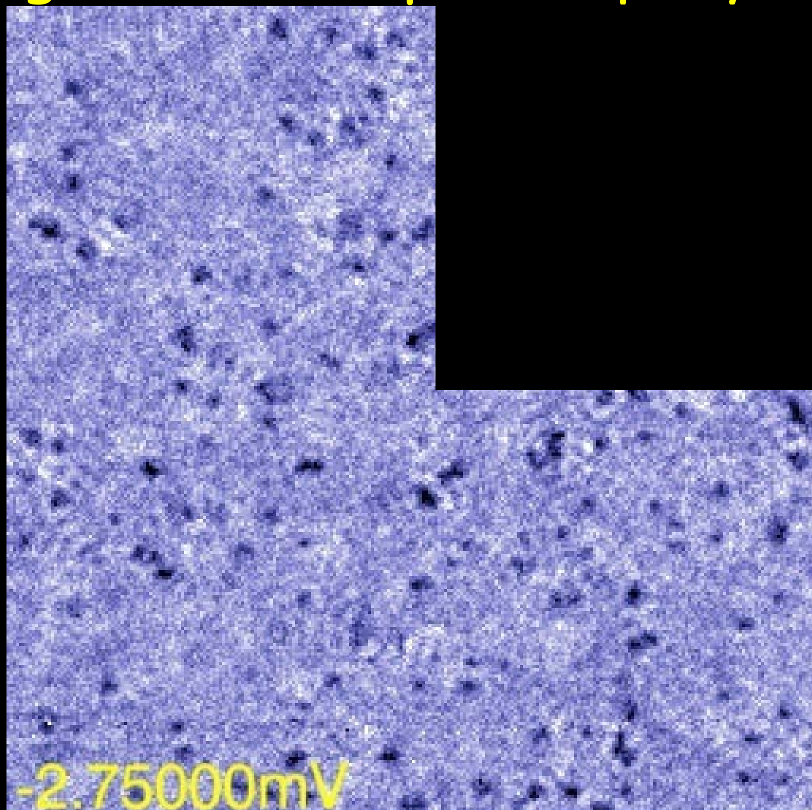
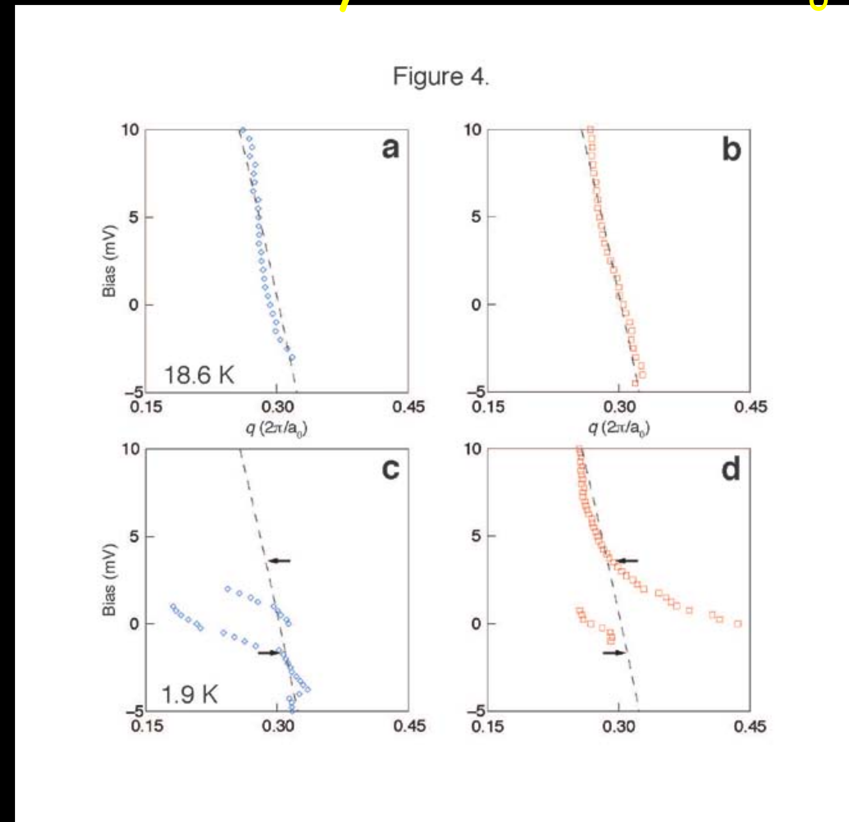
Light d-band splits rapidly into two heavy bands below T_o





- Conventional density wave, non-dispersive modulations at ***Q**** should appear in the gap-edge states both above and below E_F.. But the high-DOS gap-edge states of 'hidden order' state are at a completely different ***k***-space locations
- Instead, light band crossing E_F near ***k*** $= 0.3(\pi/a_0)$ above T_o which undergoes rapid temperature changes below T_o.
- The result is its splitting into two far heavier bands widely separated in ***k***-space and with quite different anisotropies
- The ***k***-space hybridization gap and the DOS(E) changes detected in ***r***-space occur within the same narrow energy range (consistent with the energy ranges deduced from thermodynamics and other spectroscopies),

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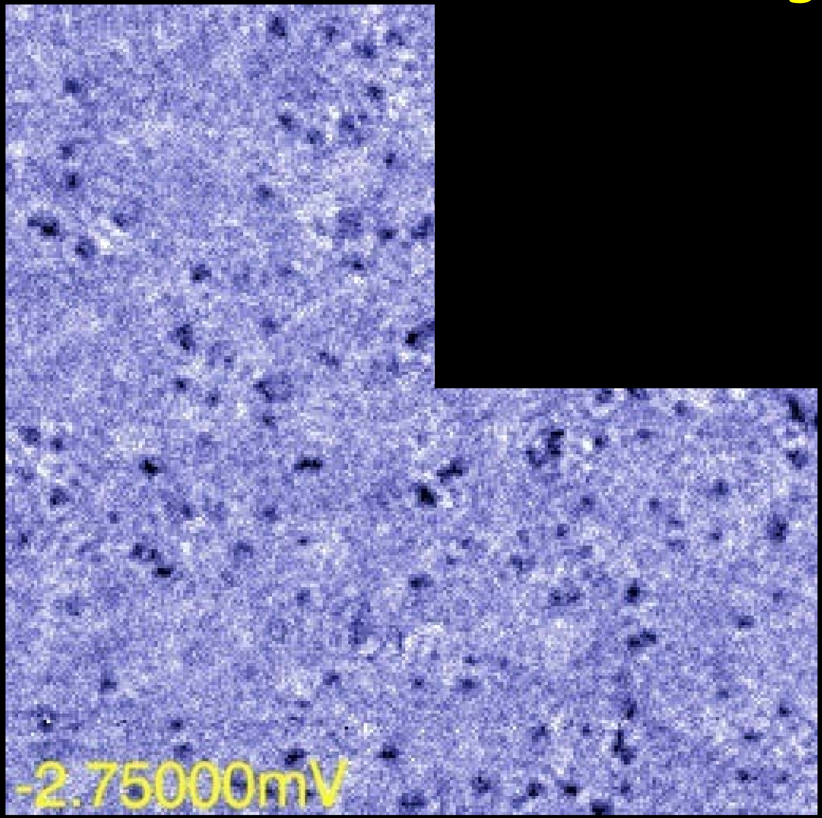
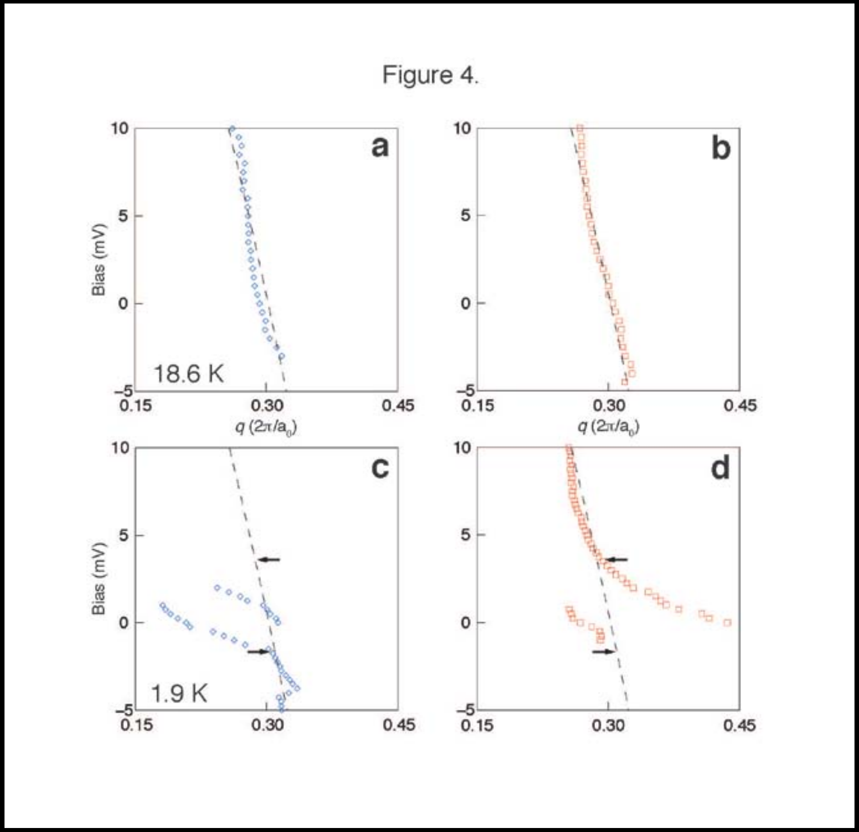
'Hidden Order' State - Change in Kondo Effect at U atoms





'Hidden order' transition is caused primarily by a sudden alteration of the many-body state centered upon each U atom, with associated alterations to the ***r***-space /***k***-space hybridization processes

A.R. Schmidt *et al* (2009)