Towards Room Temperature T_c: Lessons from the "115" Materials

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LANL

Los Alamos NATIONAL LABORATORY EST. 1943

NNSA

Outline

- An advertisement:
  "Basic Research Needs for Superconductivity"

- Towards Room Temperature T_c

  $CeIn_3$ → $CeCoIn_5$ → $PuCoGa_5$?→? $(f/d)_a(M,M')_b(X,X')_c$
  (200 mK) (2.3 K) (18.5 K) (~200 K)

- Examples
  CeM_2X_2
  "115" → $NpPd_5Al_2$ (Aoki et al.)

- Towards material as an implicit parameter
  Structures that "like" to superconduct
  Role of electronic anisotropy, spin fluctuation scale

BES Workshop Report

Electricity is our most effective energy carrier

- *Clean, versatile, switchable power anywhere*

Power grid cannot meet 21st century challenges

- *Capacity, reliability, quality, efficiency*

Superconducting technology is poised to meet the challenge

Present generation materials enable grid connected cables and demonstrate control technology

Basic and applied research needed to lower cost and raise performance

High risk-high payoff discovery research for next-generation superconducting materials

- *Higher temperature and current capability*
- *Understand fundamental phenomena of transition temperature and current flow*

http://www.sc.doe.gov/bes/reports/abstracts.html#SC

Superconductivity Research Continuum

Discovery Research

- Room-temperature superconductor *(Grand Challenge)*
- Superconductors by design *(Grand Challenge)*
- Atomic scale control of materials structure and properties
- Tuning competing interactions for new phenomena
- Unravel interaction functions generating high temperature superconductivity
- Predictive understanding of strongly correlated superconductivity
- Microscopic theory of vortex matter dynamics
- Nano-meso-scale superconductivity

Use-inspired Basic Research

- **100K isotropic SC *(Grand Challenge)***
- **Achieve theoretical limits of critical current *(Grand Challenge)***
- **3-d quantitative determination of defects and interfaces**
- **Intrinsic and intentional inhomogeneity**
- **"Pinscape engineering" and modeling of effective pinning centers**
- **Next Generation SC wires**

Applied Research

- Technology Milestones:
  - **2G coated conductor carrying 300 A x 100 m (2006)**
  - **In-field performance for 50 K operating temperature**
  - **electric power equipment with ½ the energy losses and ½ the size**
- **wire with 100x power capacity of same size copper wires at $10/kiloamp-meter.**
- **Assembly and utilization R&D issues**
- **Materials compatibility & joining issues**

Technology Maturation & Deployment

- Cost reduction
- Scale-up research
- Prototyping
- Manufacturing R&D
- Deployment support

Office of Science
BES

Technology Offices
EDER

Next Generation Materials

~ 50 copper oxide superconductors

Highest Tc = 164 K under pressure

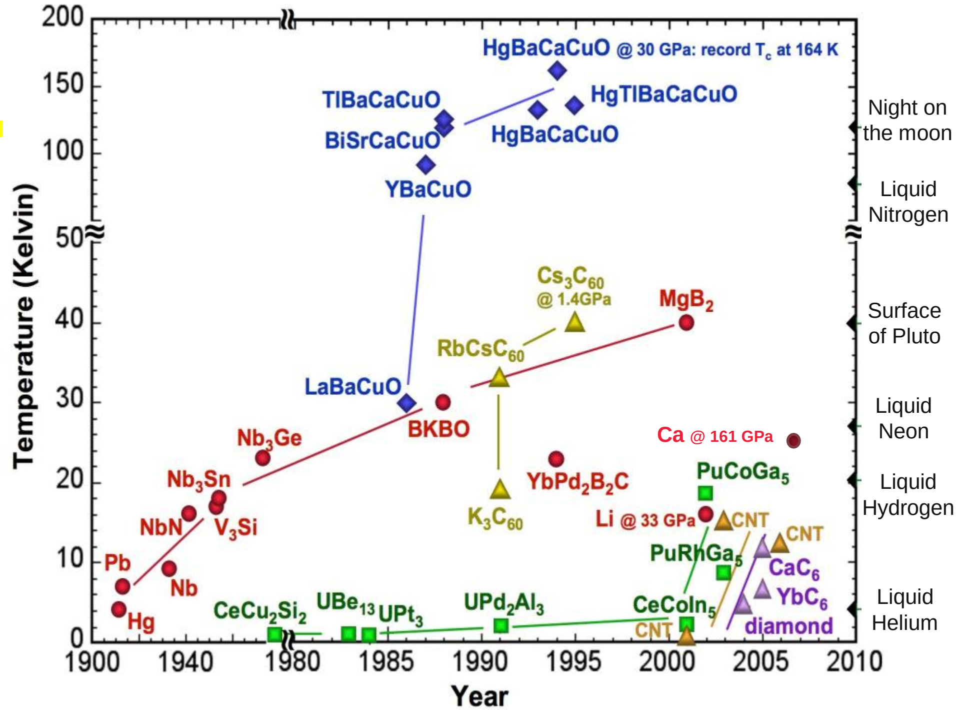
(1/2 Room Temp)

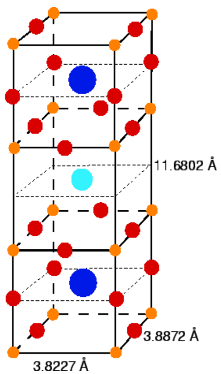
Only class of high T_c superconductors ?

High T_c superconductors $\geq$ 4 elements

55 superconducting elements

-> 55^4 ~ 10 million quaternaries





Search strategies for new superconductors

- Quaternary and higher compounds
- Layered structures
- Highly correlated normal states
- Competing high temperature ordered phases

Target Properties

Higher Tc &

Jc

isotropy

Ductility

…

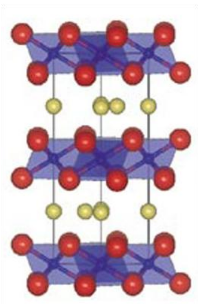
Challenge

Discover next generation complex superconductors

Superconductors by Design

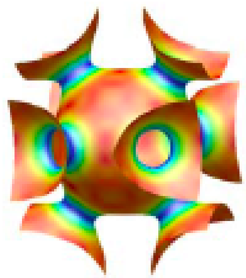
Discovery by serendipity: Hg (1911), copper oxides (1986), MgB_2 (2001), $NaCoO_2$:H_2O (2003)

Discovery by empirical guidelines: competing phases, layered structures, light elements, . . .
B-doped diamond (2004), CaC_6 (2005)



Crystal Structure
Composition

+



Electronic Structure
Density functional theory

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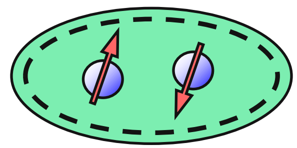
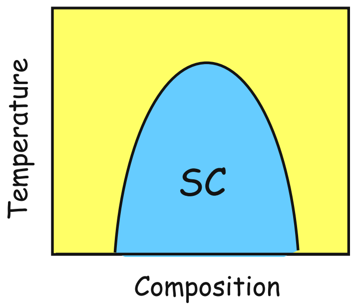


Pairing Mechanism
phonons (classical BCS)
spin fluctuations
valence fluctuations

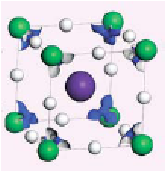
=



Superconductivity

Computationally designed superconductors

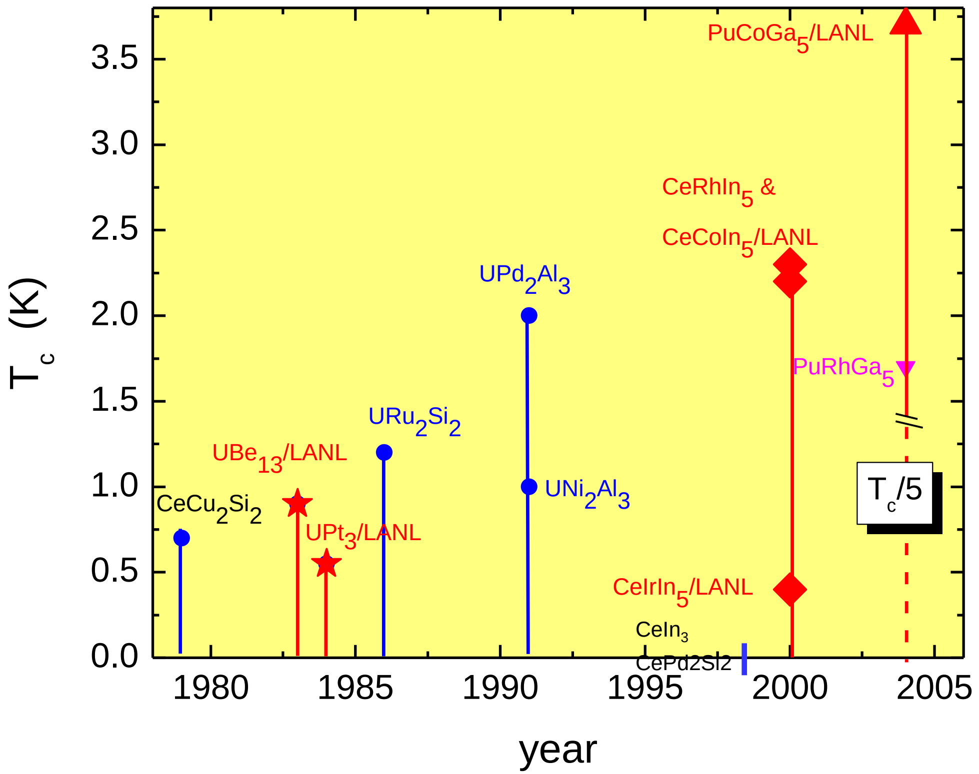
- Electronic structure calculation by density functional theory
- Large scale phonon calculations in nonlinear, anharmonic limit
- Formulate "very strong" electron-phonon coupling (beyond Eliashberg)
- Determine quantitative pairing mechanisms for high temperature SC



J. Mater. Chem., 2006
Computed metal hydride superconductor

Challenge: Create a paradigm shift to superconductors by design

Known Heavy Fermion Superconductors



Growing number of HF SCs in recent years:

The originals:
UBe_{13}, UPt_3, URu_2Si_2, UNi_2Al_3, UPd_2Al_3

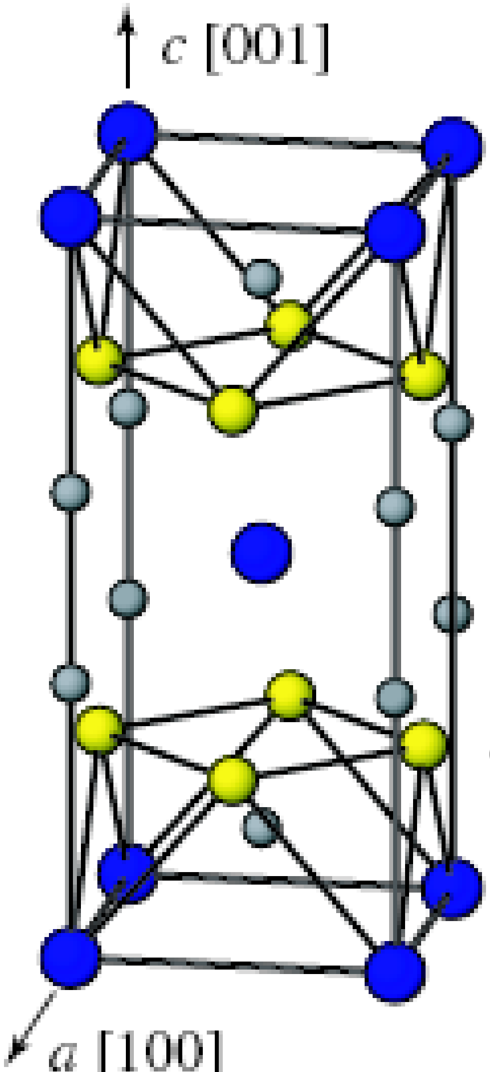
Nearly ferromagnetic:
UGe_2, URhGe

Nearly antiferromagnetic:
$CeCu_2Si_2$ and related
$CeRhIn_5$ and related

$PuCoGa_5$, $PuRhGa_5$, $NpPd_5Al_2$

$PrOs_4Sb_{12}$, $CePt_3Si$, …

CeM_2X_2



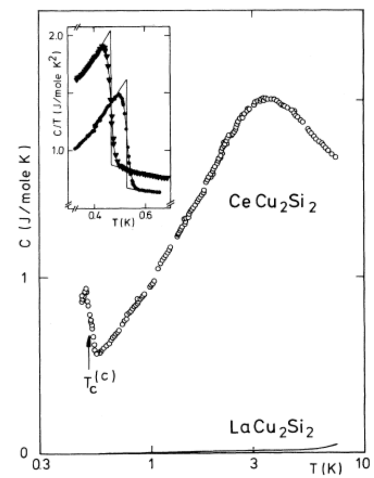
(blue) Ce

(gray) X=Si, Ge

(yellow) M=Cu, Pd, Rh

TABLE I. Properties of superconducting CeM_2X_2

Material	T_c (K)	V ($Å^3$)[a]	P_c^{obs} (kbar)[b]
$CeCu_2Si_2$	0.64	167.4	0
$CeRh_2Si_2$	0.35	169.8	9 ± 1
$CePd_2Si_2$	0.50	177.0	27 ± 2 (Ref. 8)
$CeCu_2Ge_2$	0.60	177.7	77 ± 2 (Ref. 7)



Steglich (1979)

CeM_2X_2 – Pressure Tuning

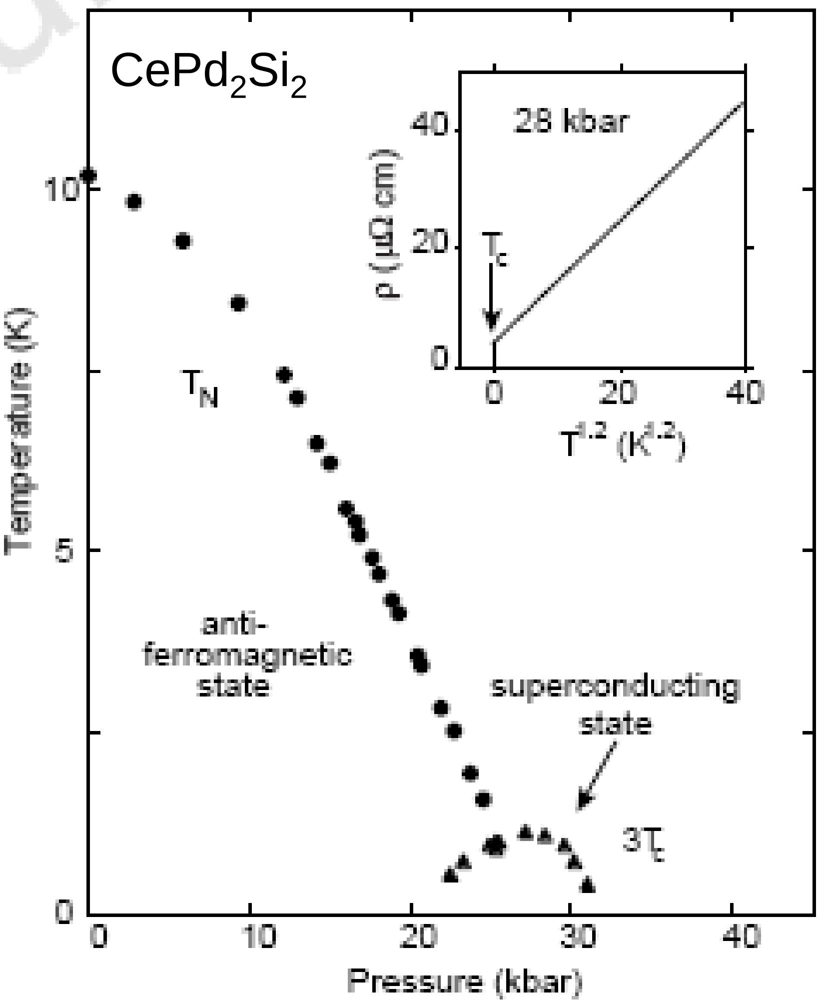
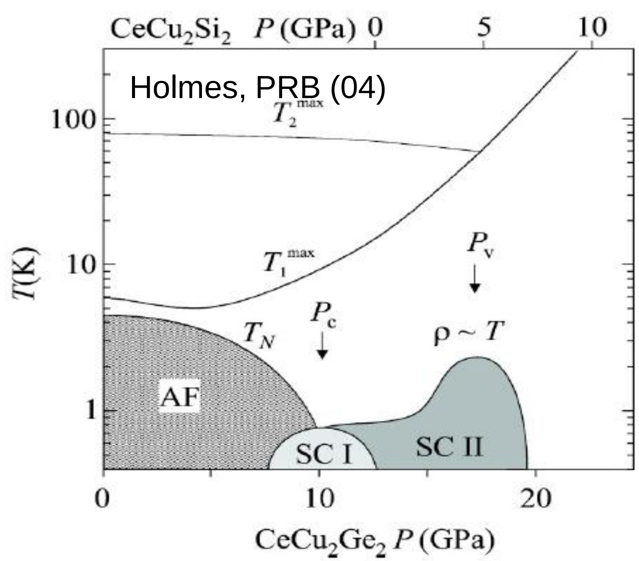
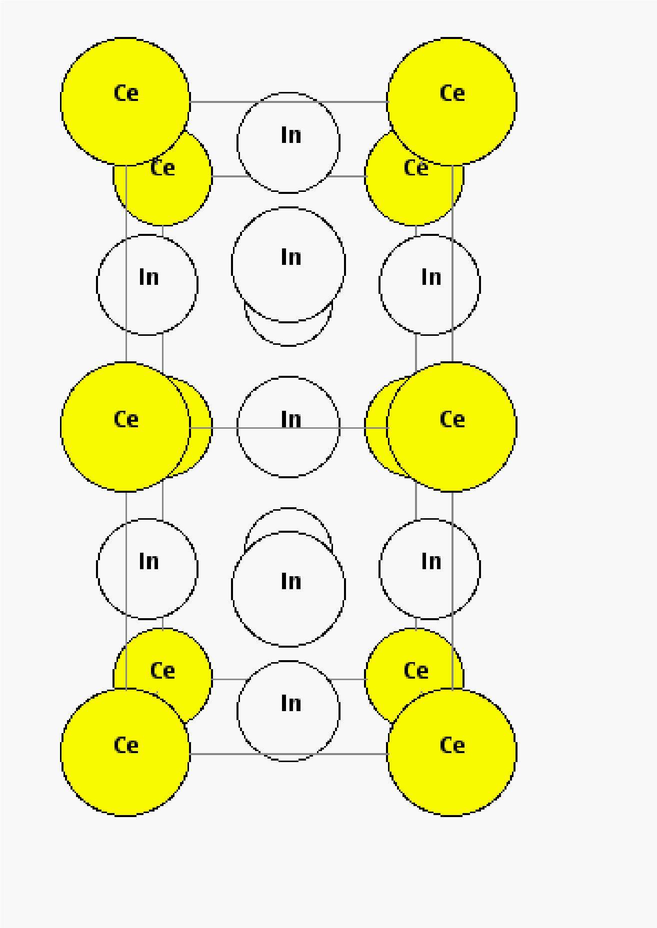


TABLE I. Properticompounds.

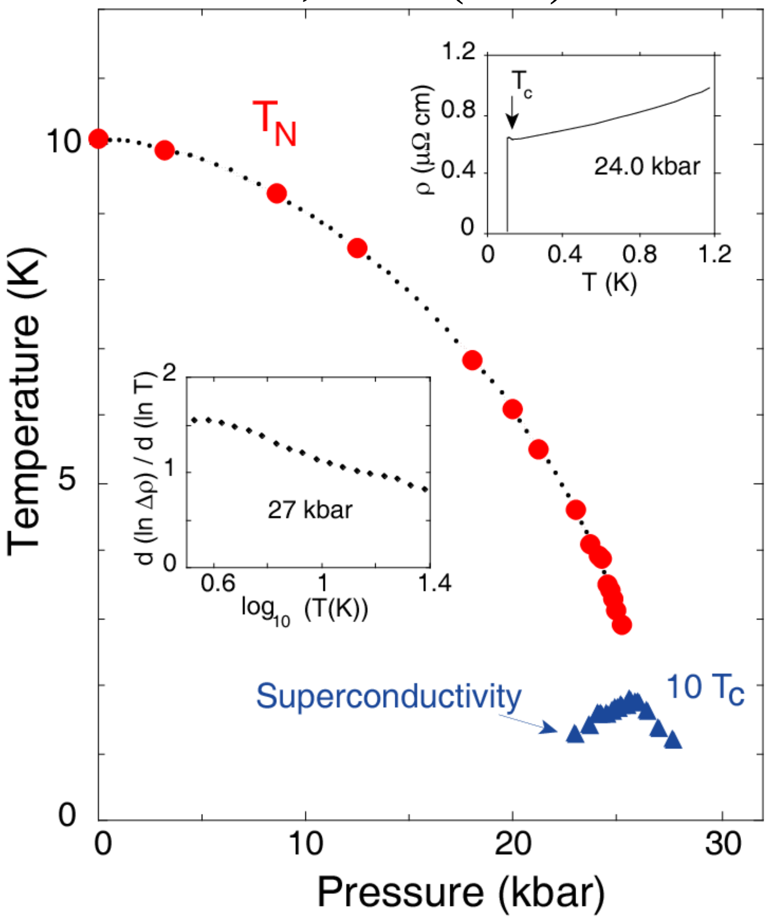
Material	T_c (K)	V_c^{calc} ($Å^3$)[c]
$CeCu_2Si_2$	0.64	167.4
$CeRh_2Si_2$	0.35	168.3
$CePd_2Si_2$	0.50	172.2
$CeCu_2Ge_2$	0.60	164.0



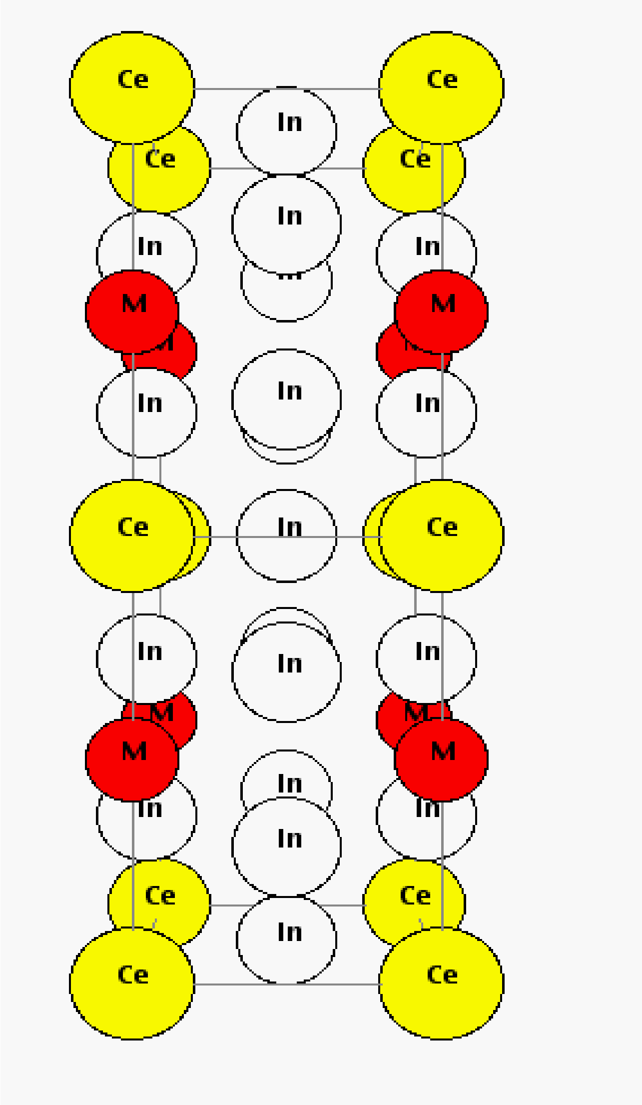
$CeIn_3$



Mathur, Nature (1998)



$CeMIn_5$



M = Co, Rh, Ir (isovalent)

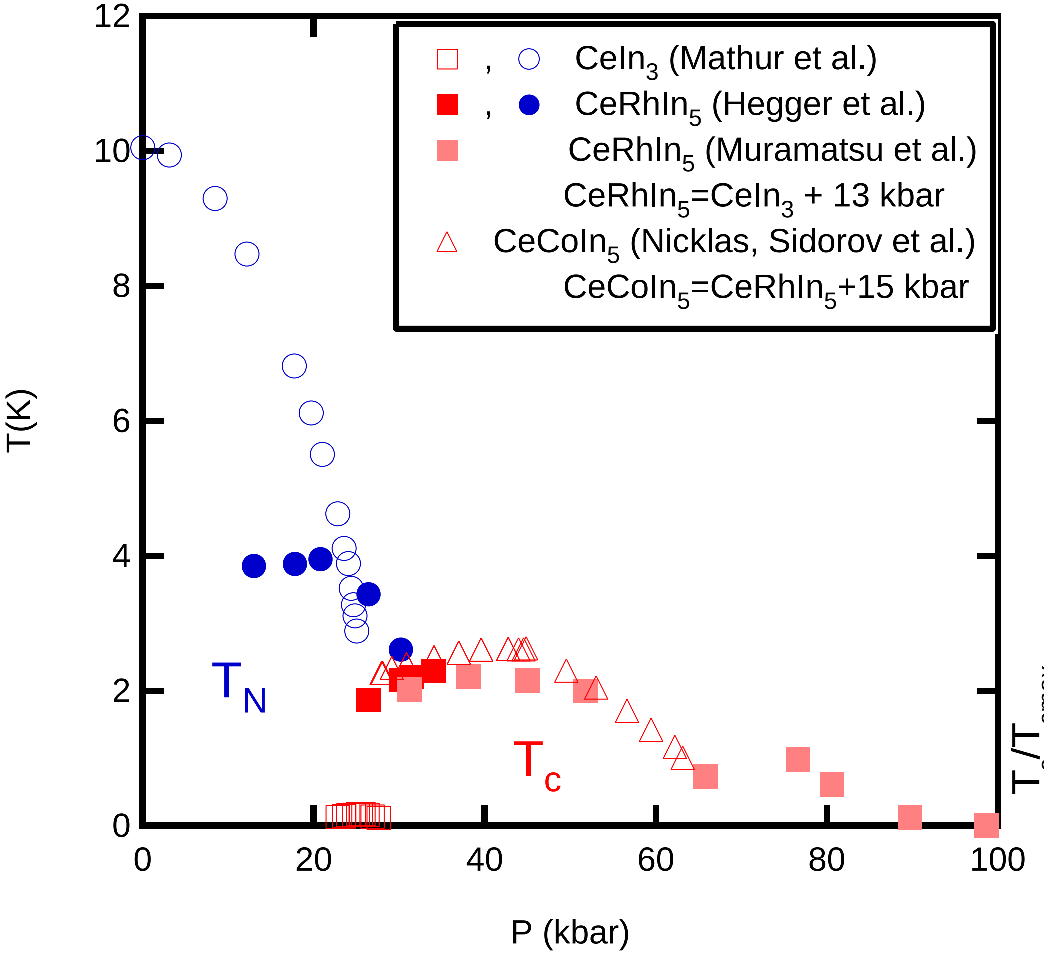
A layered version of $CeIn_3$?

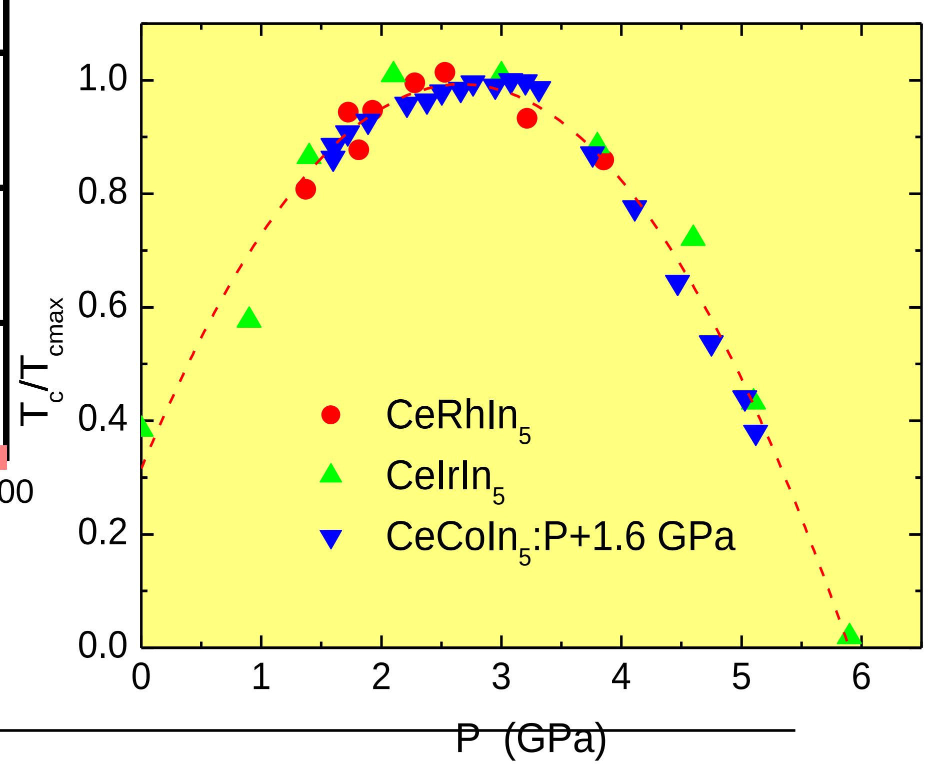
$CeRhIn_5$: 3.8 K AFM

$CeCoIn_5$: 2.3 K SC

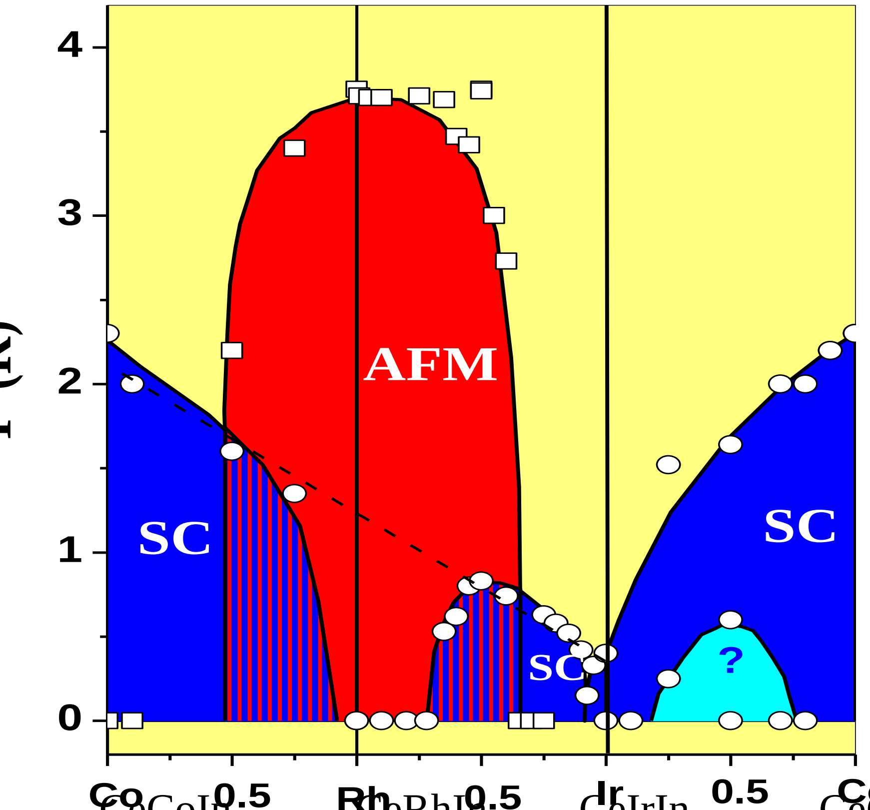
$CeIrIn_5$: 0.4/1.0 K SC

$CeMIn_5$ – Pressure Tuning

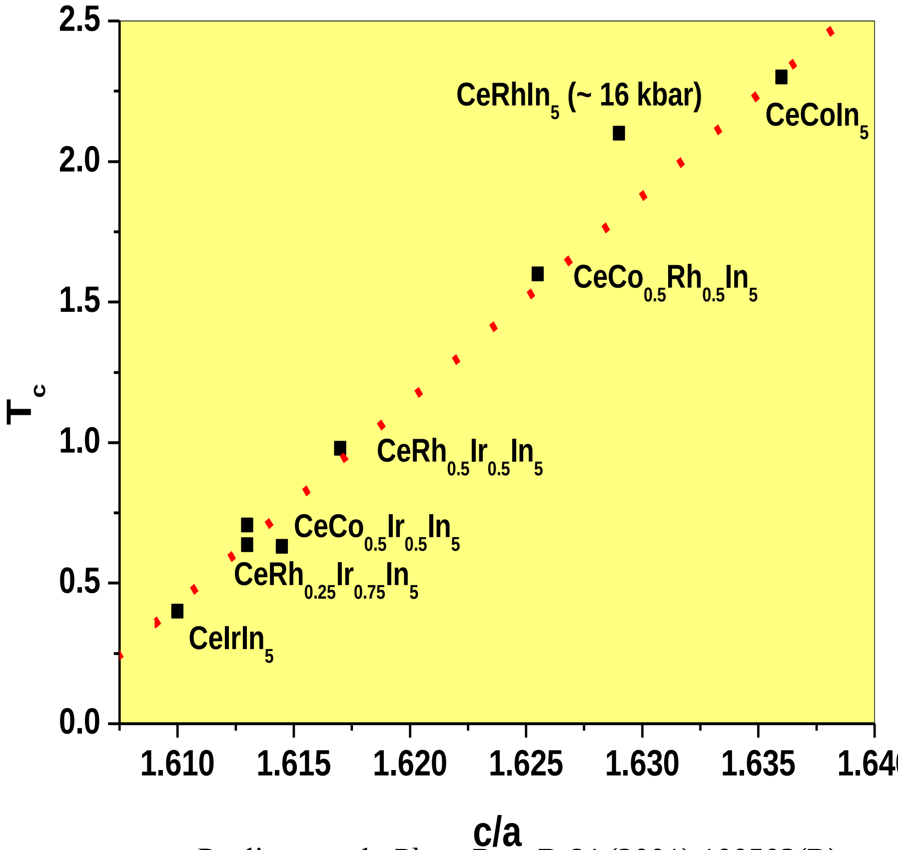




$CeMIn_5$ – Chemical Substitution

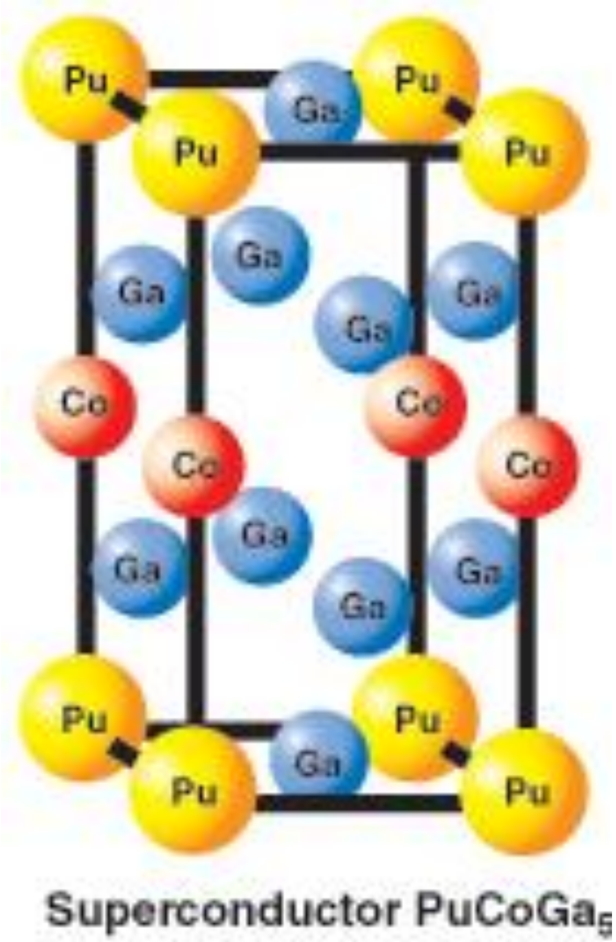


$CeCoIn_5$ $CeRhIn_5$ $CeIrIn_5$ $CeCoIn_5$

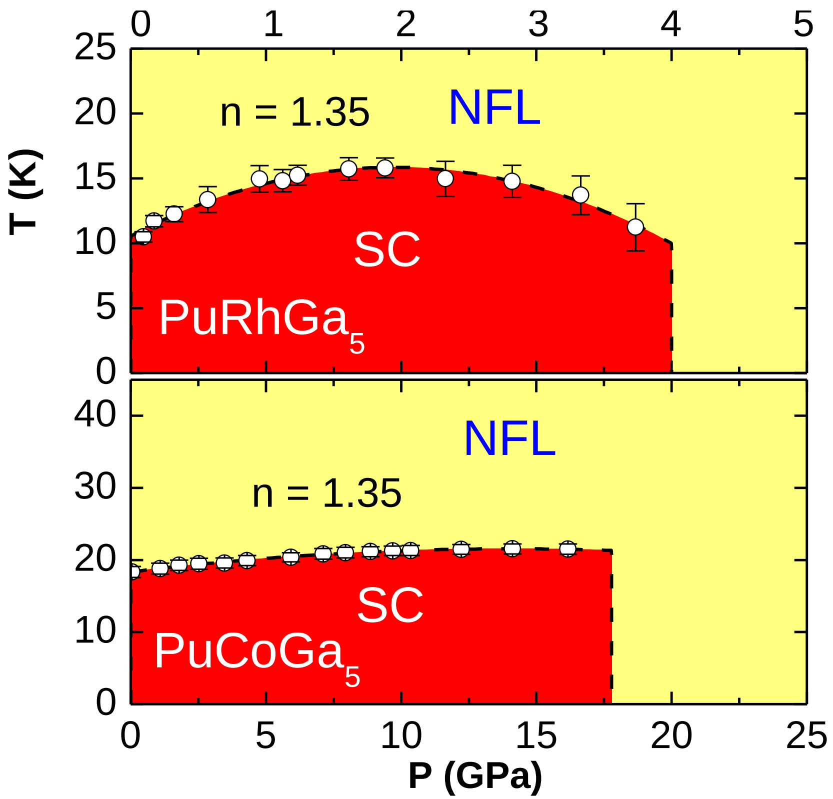


Pagliuso et al., Phys. Rev. B 64 (2001) 100503(R)

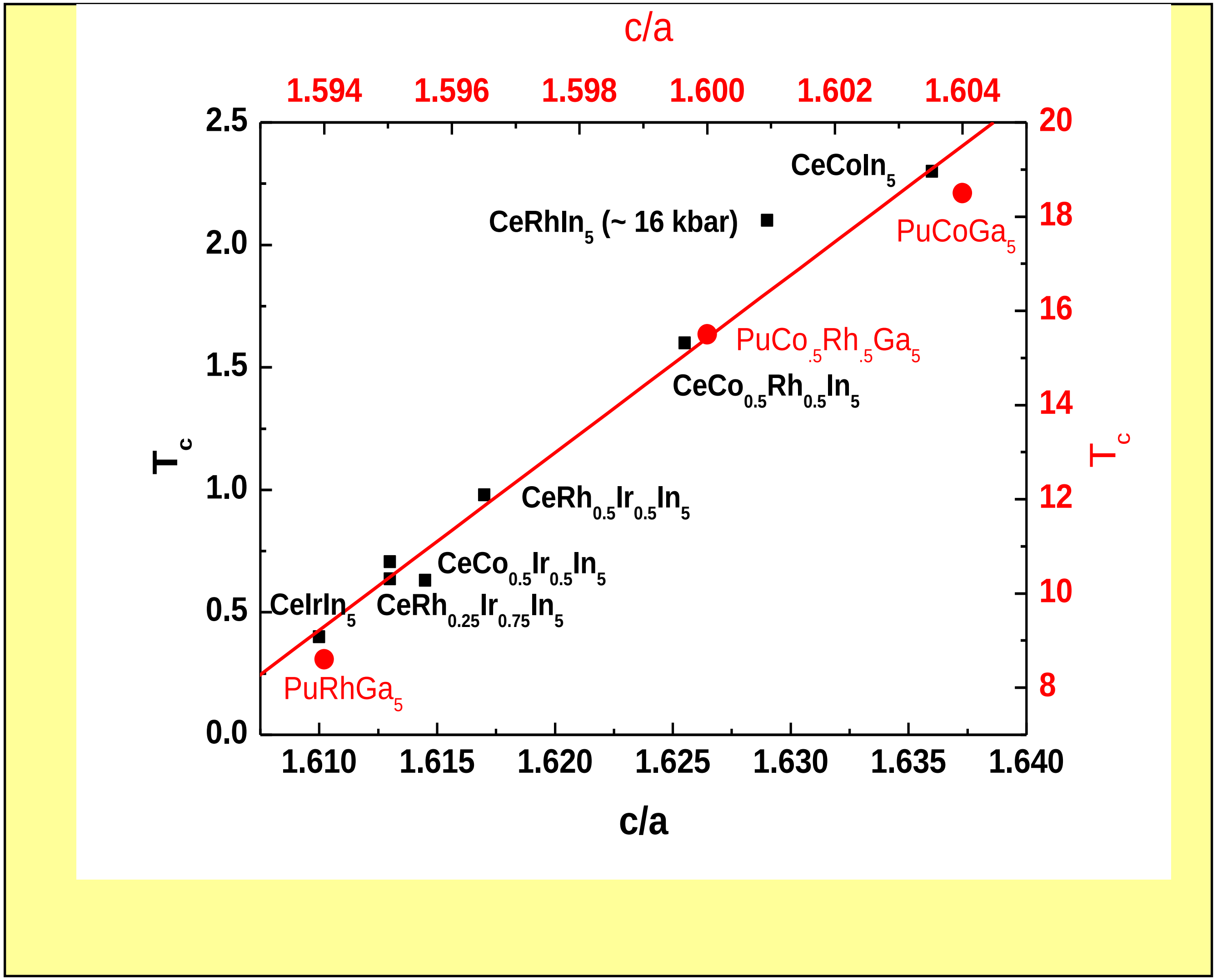
$PuMGa_5$



$PuCoGa_5$: 18.5 K SC
$PuRhGa_5$: 9 K SC

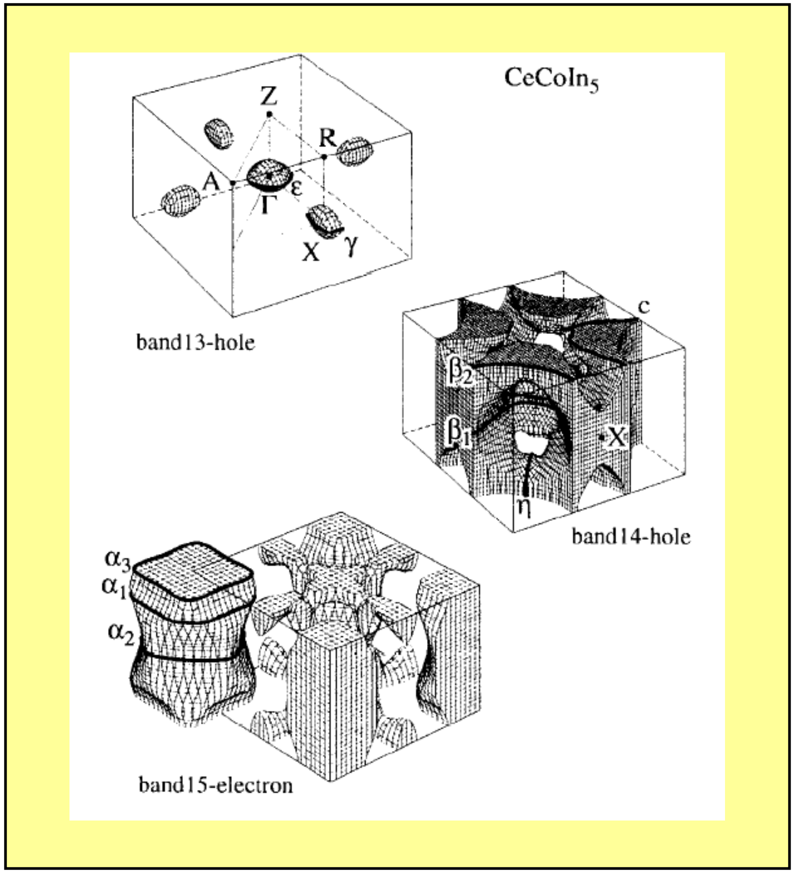


T_c and c/a: anisotropy tuning

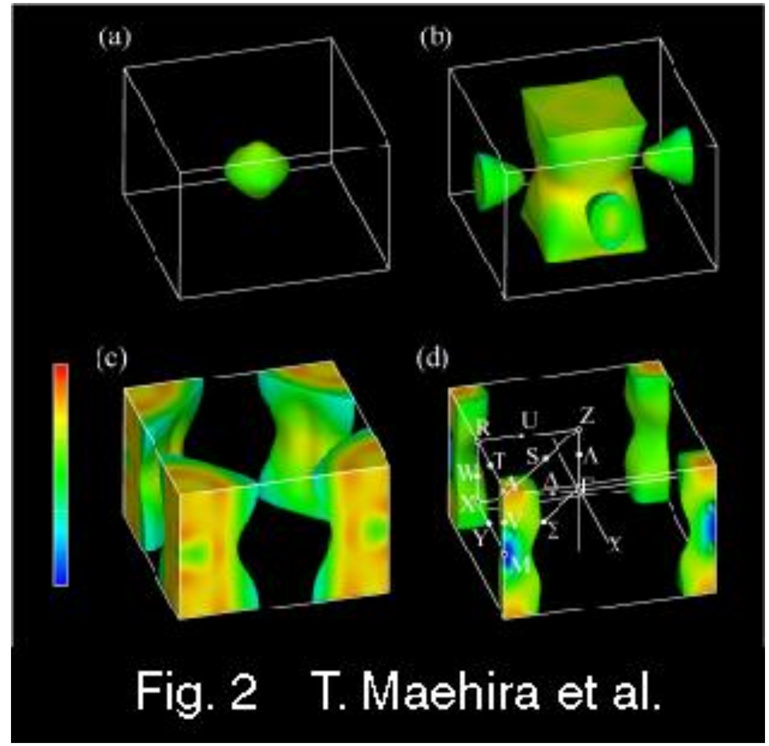


E.D. Bauer et al., PRL 93 (2004) 147005

Electronic Anisotropy: Quasi-2D Fermi Surface



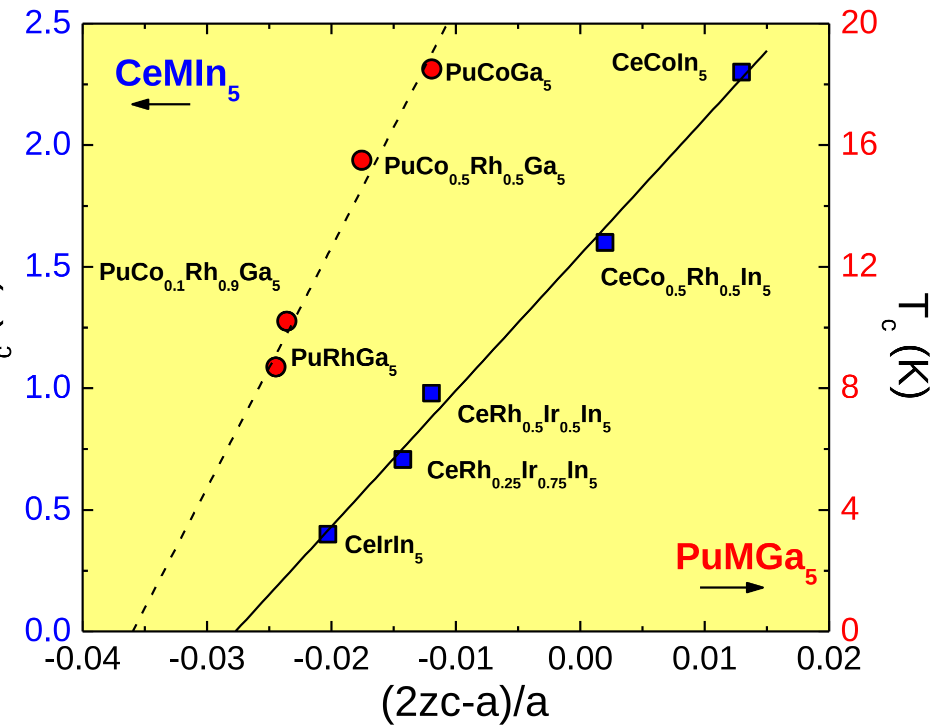
R. Settai et al., JPCM **13**, L627 (2001)

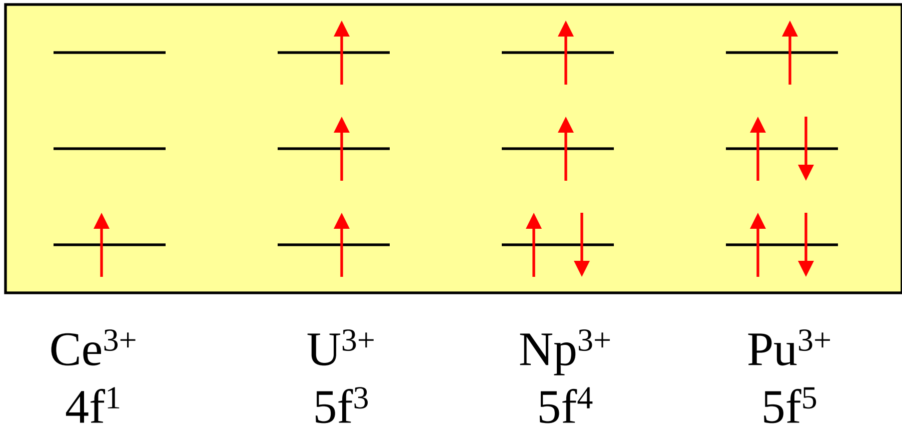


T. Maehira et al., PRL 90 (2003) 207007;
I. Opahle and P. M. Oppeneer, PRL 90 (2003) 157001

Experimentally, bulk properties (H_{c2}, ρ, χ) have anisotropies of 3 - 5

Structural distortion: Crystal-field tuning





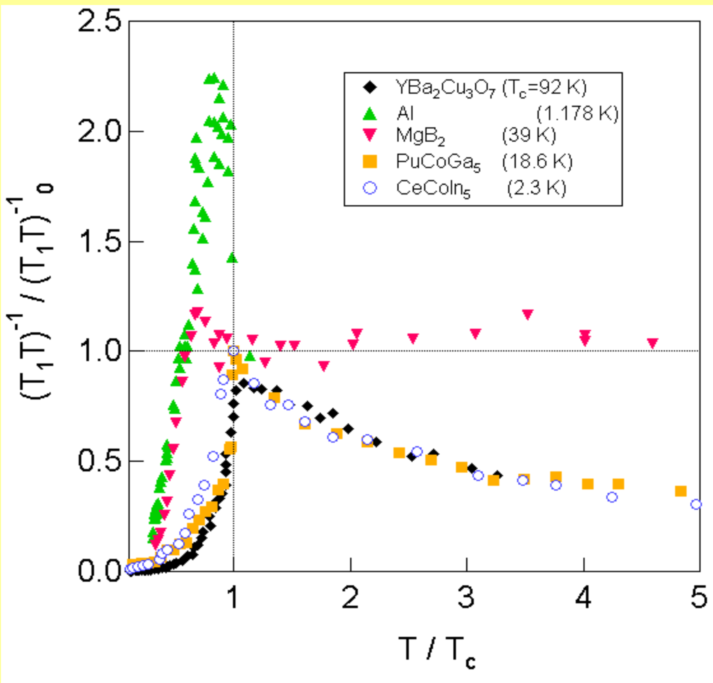
$CeMIn_5$: T_c=1.6 + 56(2zc-a)/a

$PuMGa_5$: T_c=28.4 + 790(2zc-a)a

$UMGa_5$: Kaneko, PRB 68 (2003)
Similar trends in $NpMGa_5$

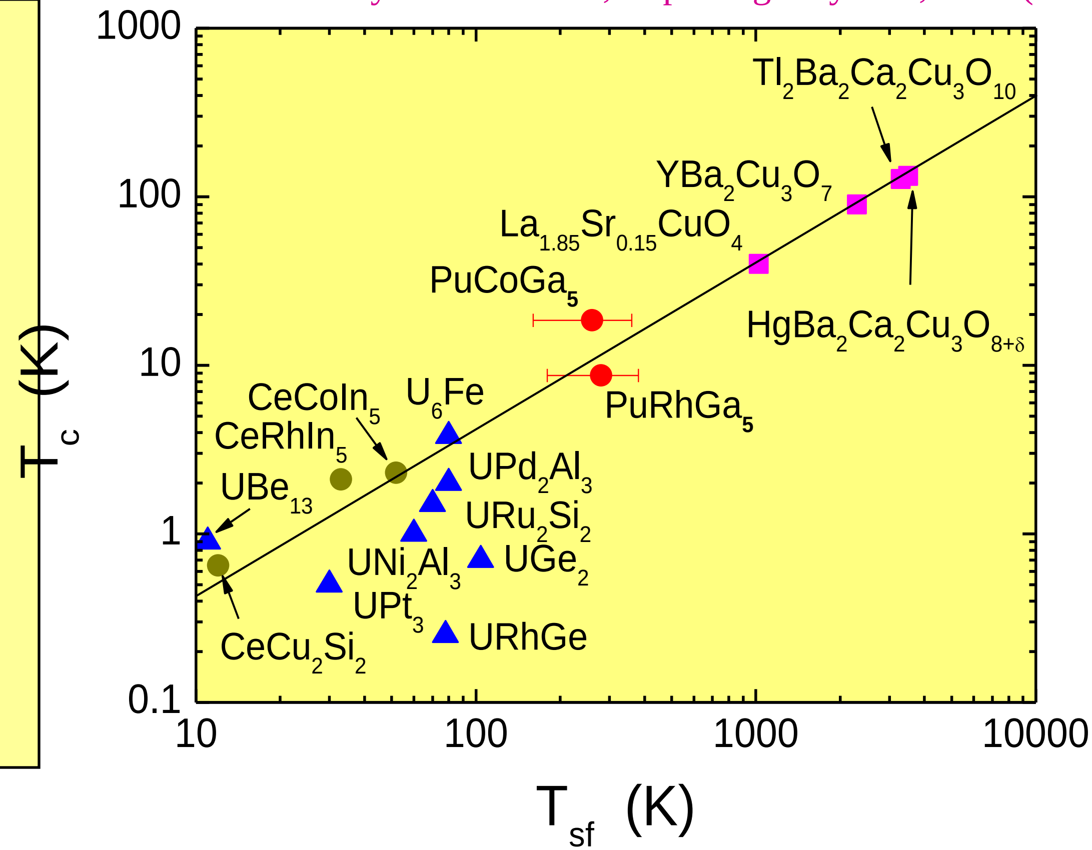
	(2zc-a)/a	T_N
UGa_3	=0	65 K
$UNiGa_5$	-1.5%	86
$UPdGa_5$	-5.1%	30
$UPtGa_5$	-7.0%	26

$PuCoGa_5$: Tuning spin fluctuations?



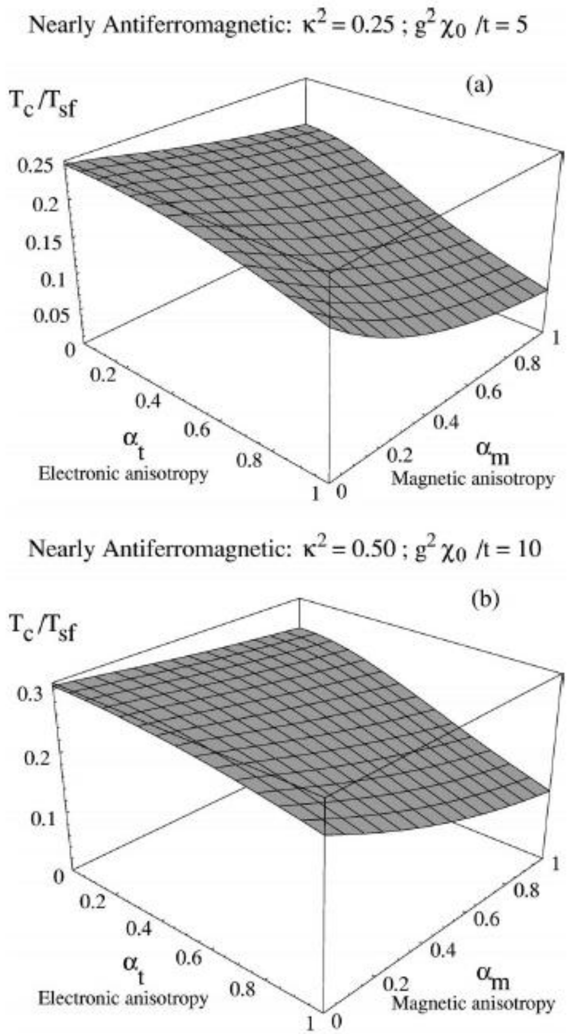
N. J. Curro et al., Nature **434**, 622 (2005).

after T. Moriya and K. Ueda, Rep. Prog. Phys. **66**, 1299 (2003)



(T_{sf} estimated from C/T for f-electron materials
and from T-linear resistivity of cuprates--Moriya and Ueda)

Model Calculations – Combining Effects



Monthoux & Lonzarich PRB (02)

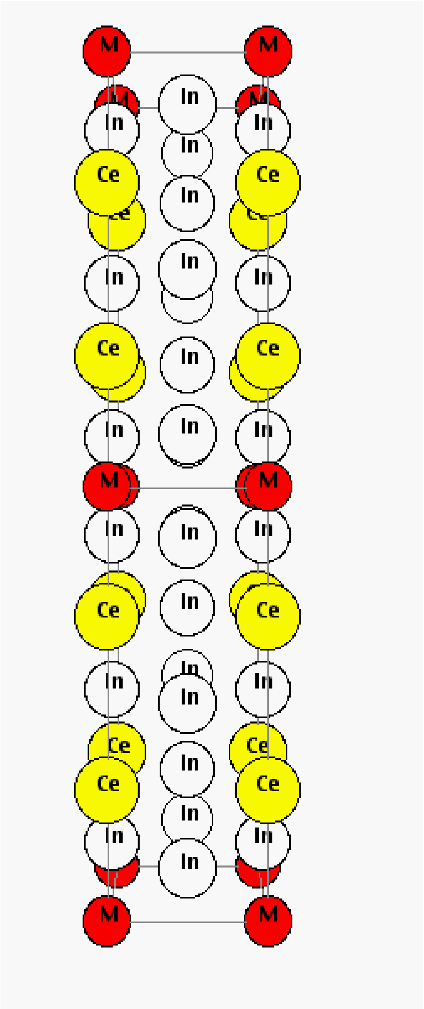
Model:
α_t = 0, quasi-2d electronic structure
= 1, cubic lattice

α_t = 0, quasi-2d magnetic correlations
= 1, 3d magnetic correlations

Similar contours for varied coupling constants
T_c(nearly AFM) ~ 10x T_c(nearly FM)

Experimentally,
T_c/T_{sf} ~ 0.05 – 0.1, $CeCoIn_5$ or $PuCoGa_5$

Increasing Anisotropy -Alternate stacking of 115



Ce_2MIn_8

- intermediate between $CeIn_3$ & $CeMIn_5$

-Ce-In no longer constrained to be co-planar

- sample quality less good due to stacking integrowths

Ce_2RhIn_8: 2.8 K AFM → 2K SC
Ce_2IrIn_8: heavy-fermion Pauli paramagnet
Ce_2CoIn_8: ~ 0.8 K SC

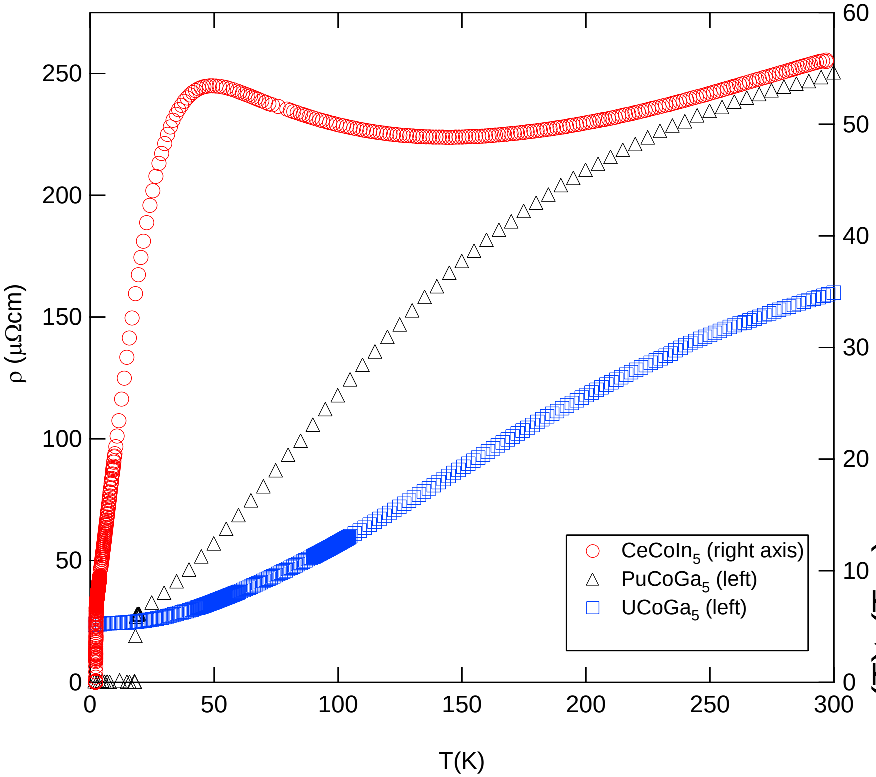
Consider bi-layers of "MIn_2" and $CeIn_3$

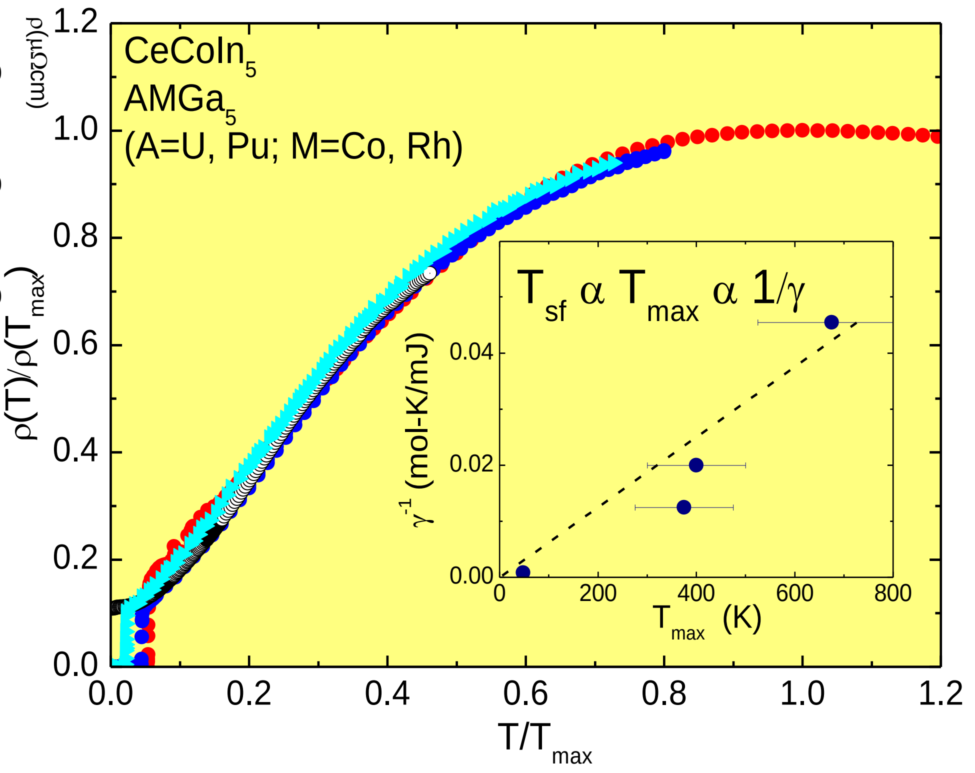
-"CeM_2In_7" ???

And same for Pu analogs

-Pu_2RhGa_8 orders antiferomagnetically

Tuning spin fluctuations (too far) - $UMGa_5$



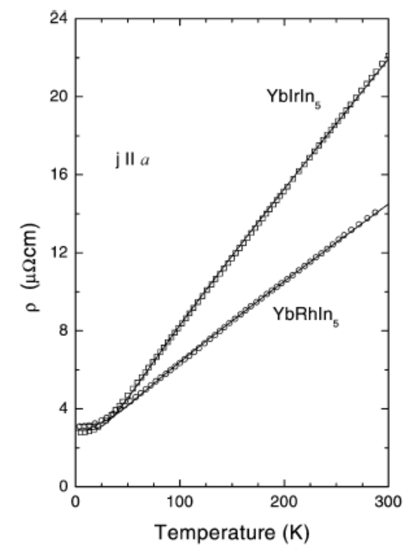


Yb-115 and Np-115

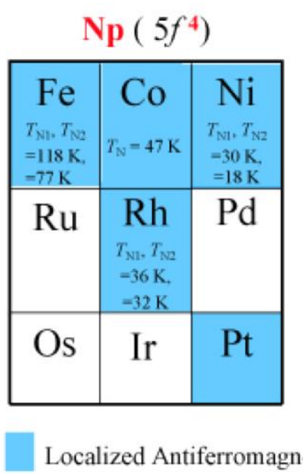
Yb^{3+} ($4f^{13}$): hole analog of Ce3+ ($4f^1$)

$YbMIn_5$ (M=Co, Rh, Ir) – good metals; divalent Yb

Pressure-induced magnetism/superconductivity??



$NpMGa_5$

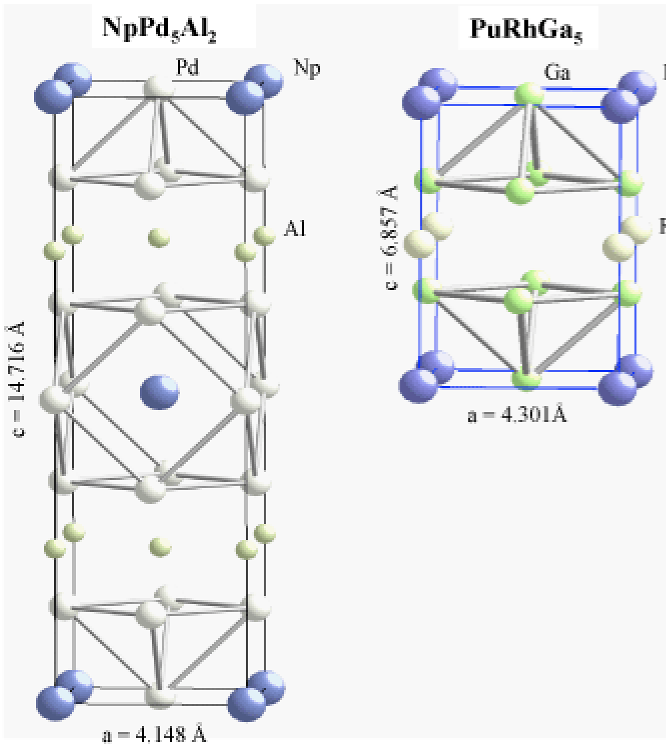


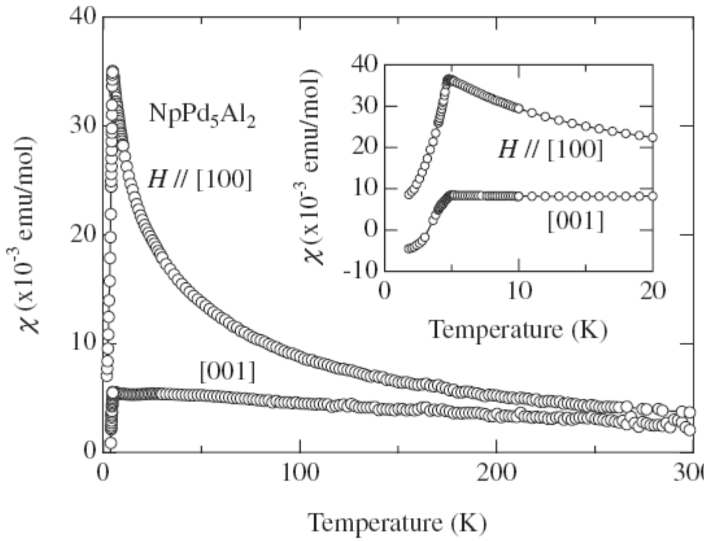
(U, Np, Pu, Am)

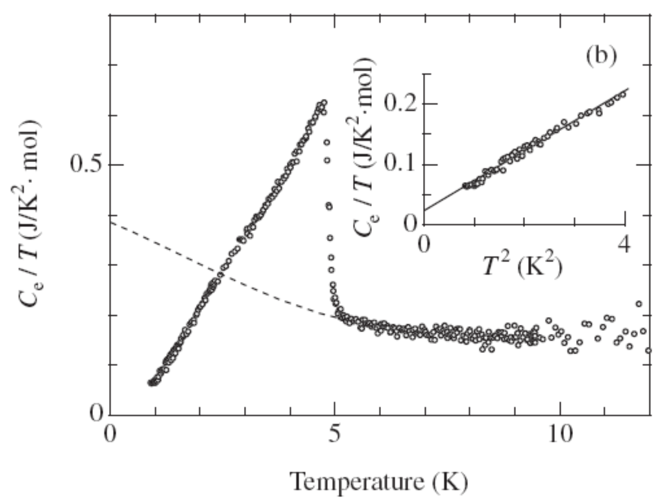
Studied extensively by Onuki group

Localized magnets, no superconductivity

$NpPd_5Al_2$ (Aoki et al., JPSJ 76 (2007) 063701)

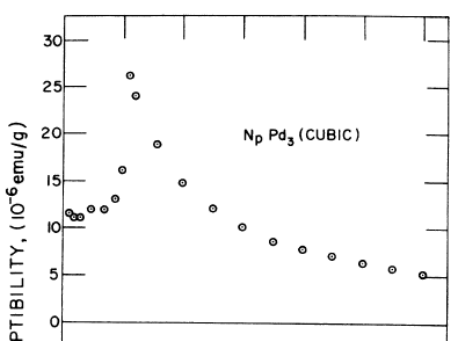




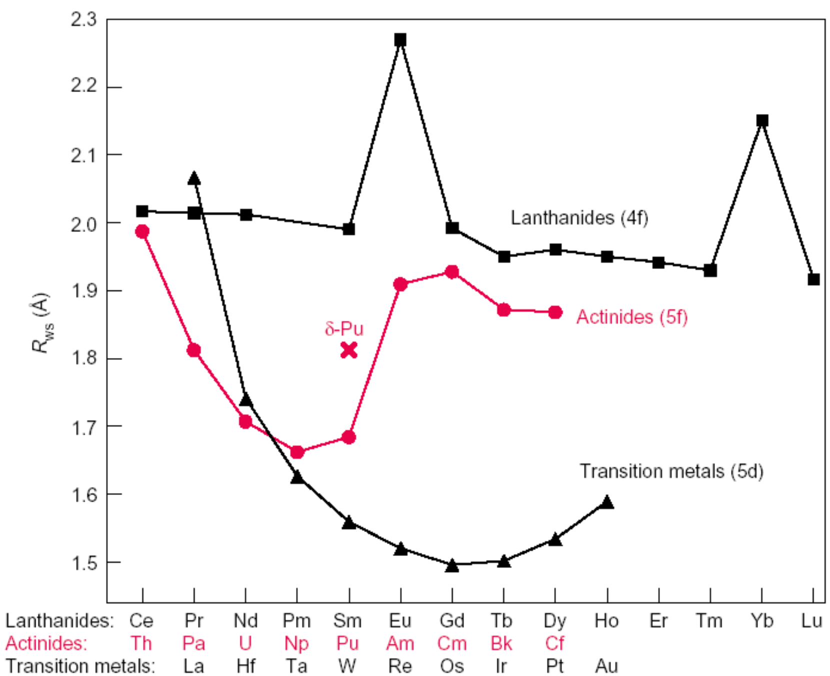


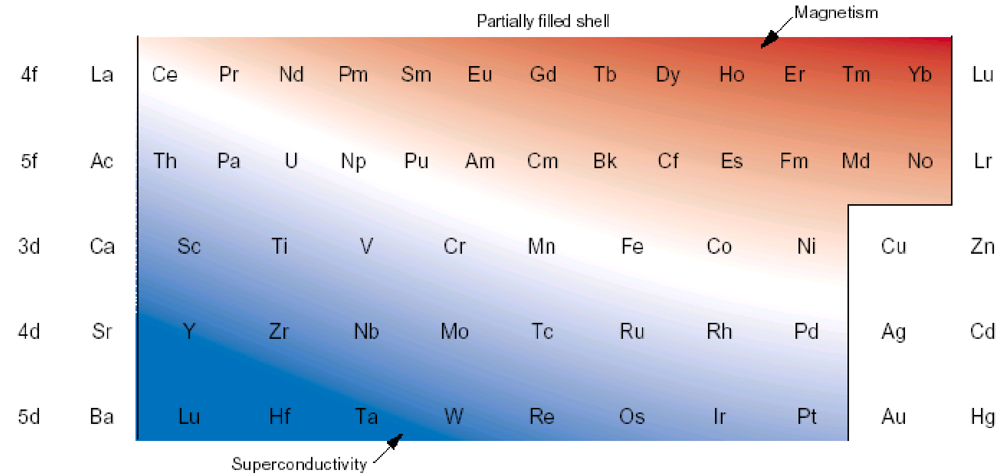
Apparent “parent compound” $NpPd_3$??

Nellis (1974)



Other transuranic compounds





Np, Pu intermetallics

- partially localized 5f electrons
- relatively unexplored phase space

Extensions to d electron metals?

Summary

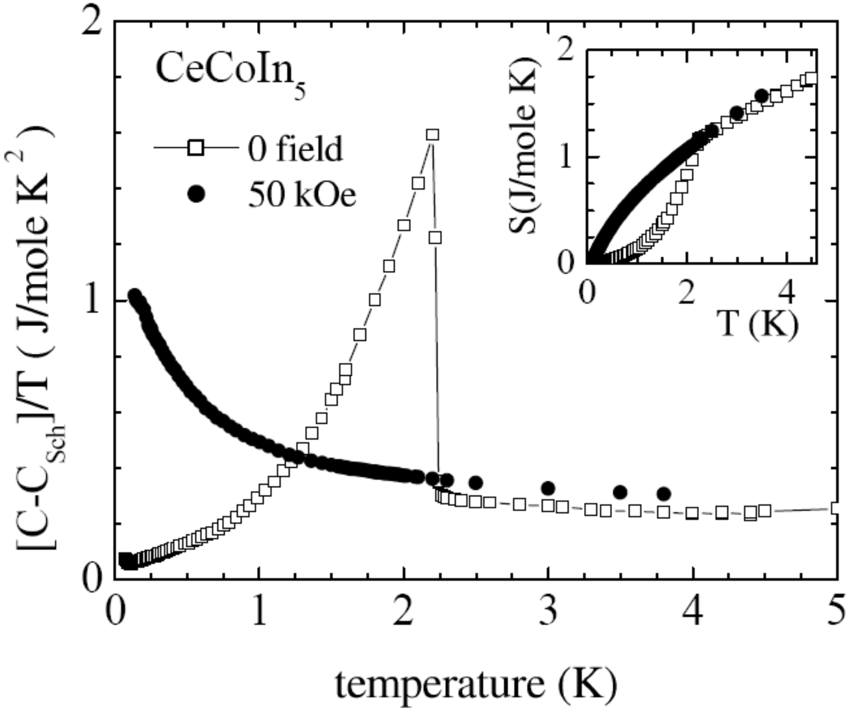
Certain crystal structures 'like' to superconduct

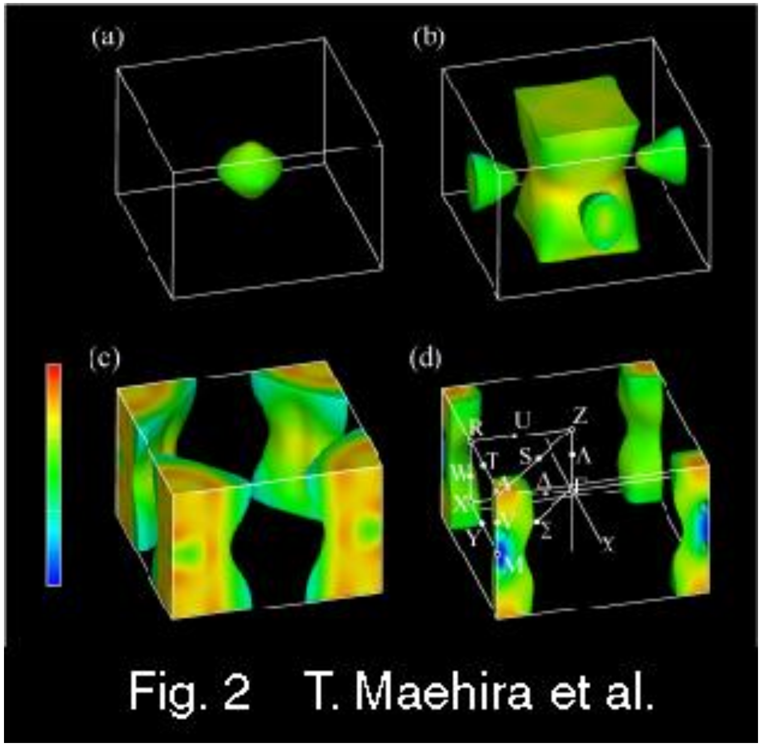
Can we calculate what's special about $ThCr_2Si_2$ and $HoCoGa_5$ structure types?

Plausible relation among $CeIn_3$ → $CeCoIn_5$ → $PuCoGa_5$

Optimistically (Naively?), perhaps there's another factor of 10 to be found through a directed random walk

Questions


CeCoIn$_5$
0 field
50 kOe
$[C-C_{Sch}]/T$ (J/mole K^2)
temperature (K)
S(J/mole K)
T (K)


(a)
(b)
(c)
(d)
Fig. 2 T. Maehira et al.