M.N.Kiselev

Strongly Correlated Systems:

High Temperature Superconductors

Heavy Fermion Compounds

Organic materials

Strongly Correlated Systems:

High Temperature Superconductors

Superconductivity: what and what for

- **Zero resistance at finite (but low) temperatures**
  - **Discovered in 1911 by Kamerlingh-Onnes (Nobel Prize in 1913): Hg superconducting at 4.2 K**
  - **Later observed in other metals like Nb, Al, … but the critical temperature, T_c<23K**

- **Applications (examples):**

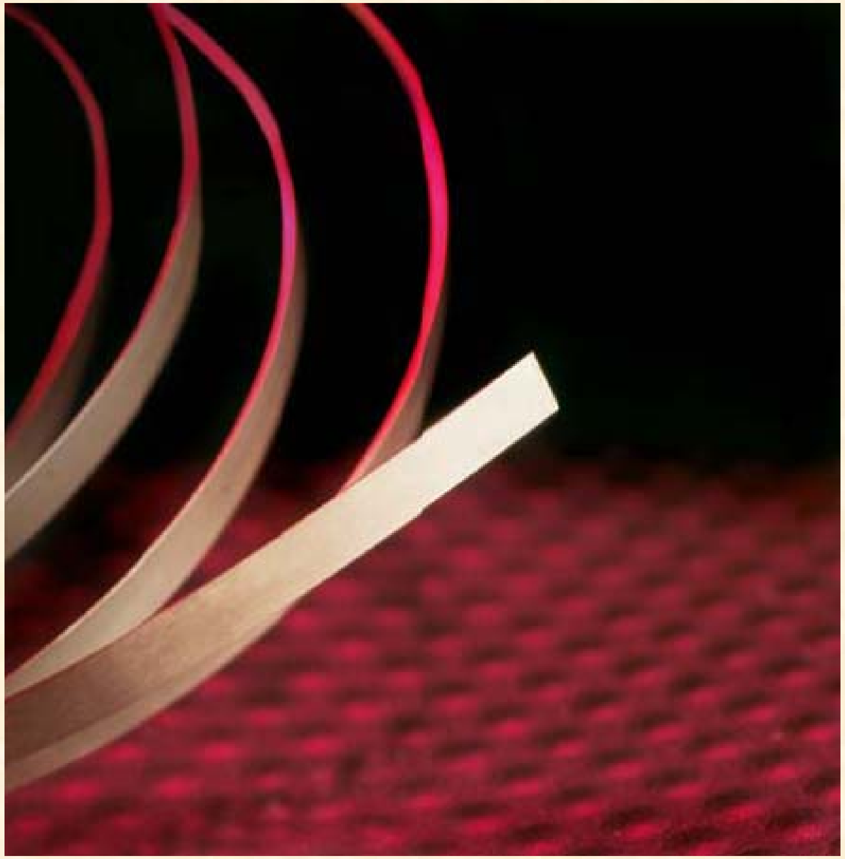
MRI (without need for liquid He cooling?)

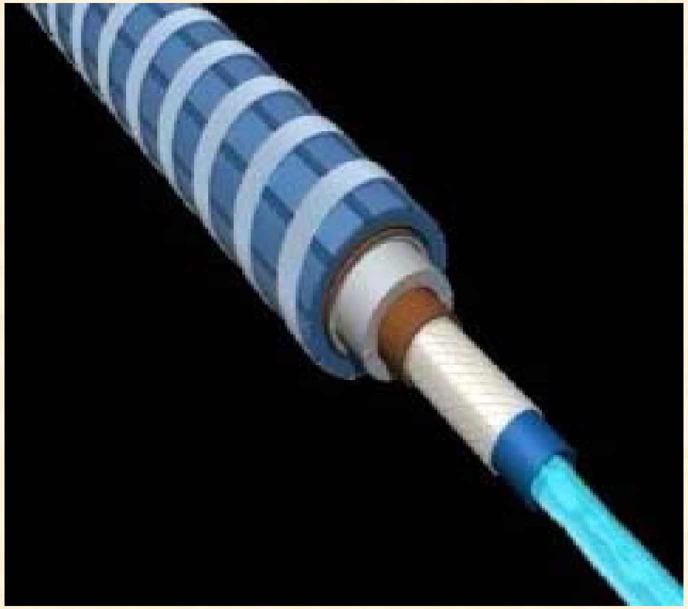
Loss free power transmission (without cooling?)

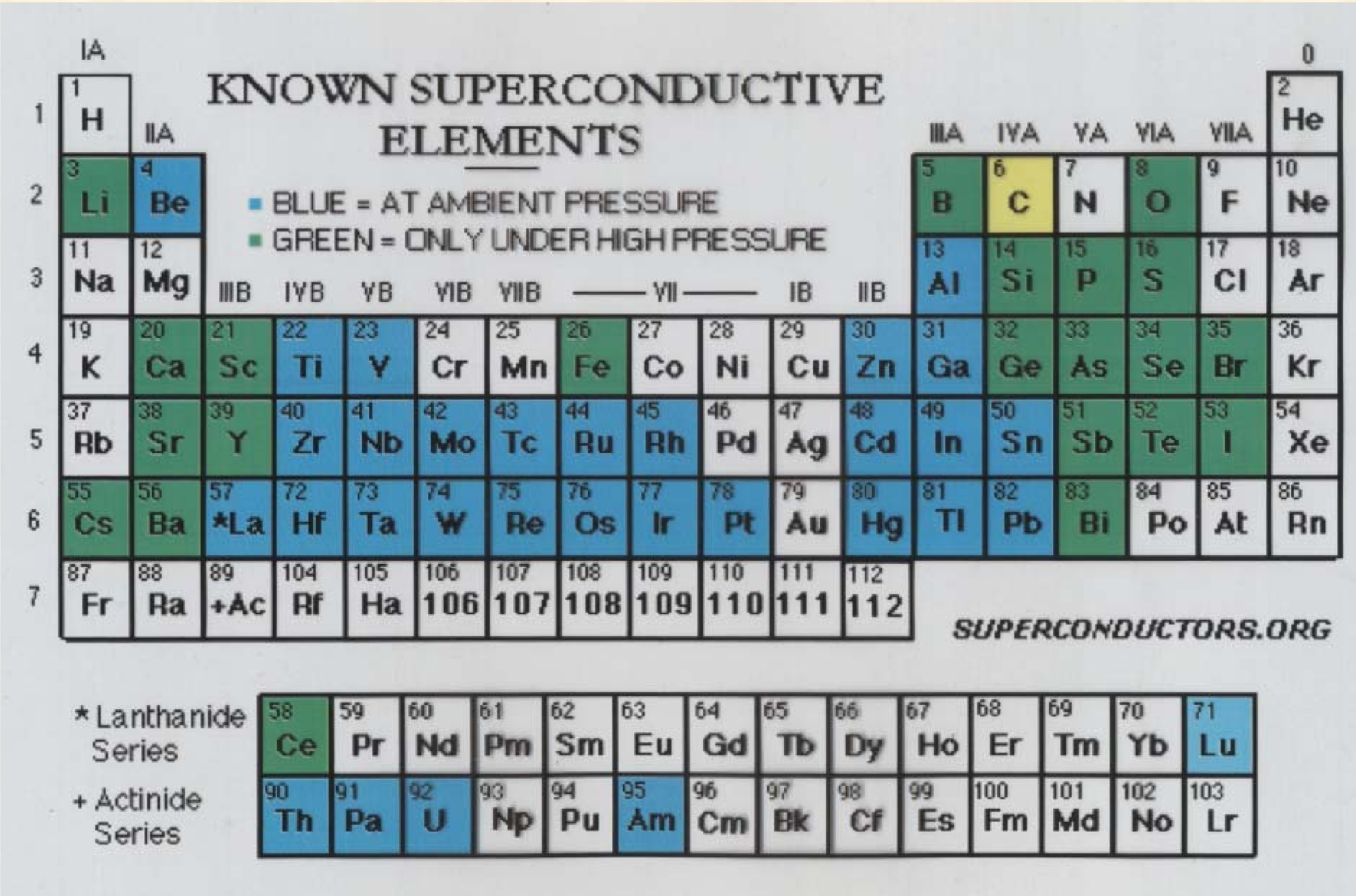
Superconducting magnetically levitated train

Superconducting magnet used to detonate mines

Superconducting Cables






KNOWN SUPERCONDUCTIVE ELEMENTS
BLUE = AT AMBIENT PRESSURE
GREEN = ONLY UNDER HIGH PRESSURE
SUPERCONDUCTORS.ORG
* Lanthanide Series
+ Actinide Series

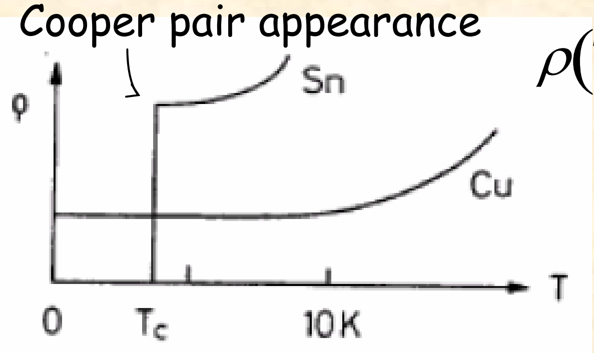
Short history of superconductivity

- 1908 Heinke Kemerlingh Onnes achieves very low temperature producing liquid He (< 4.2 K)
- 1911 Onnes and Holst observe sudden drop in resistivity to essentially zero SC era starts
- 1914 Persistent current experiments (Onnes)
- 1933 Meissner-Ochsenfeld effect observed
- 1935 Fritz and London theory
- 1950 Ginsburg - Landau theory
- 1957 BCS Theory (Bardeen, Coper, Schrieffer)
- 1962 Josephson effect is observed

- 1967 Observation of Flux Tubes in Type II superconductors (Abrikosov, Ginzburg, Leggett)
- 1980 Tevatron: The first accelerator using superconducting magnets
- 1986 First observation of Ceramic Superconductor at 35 K (Bednorz, Muller)
- 1987 first ceramic superconductor at 92 K (above liquid Nitrogen at 77 K !) HTS era starts
- 2003 discovery of a metallic compound the B_2Mg superconducting at 39 K (x2 T_c of Nb_3Sn)
  - It took ~70 years to get first accelerator from conventional superconductors.
  - How long will it take for HTS or B_2Mg to get to accelerator magnets? Have patience!

What is a superconductor

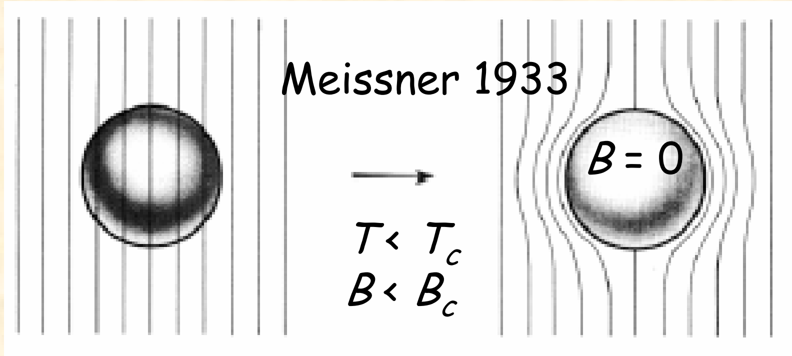
Below the *critical temperature* T_c the resistivity drops



$$\rho(T) = \rho_0 + cT^5$$

phonon-e⁻ interaction

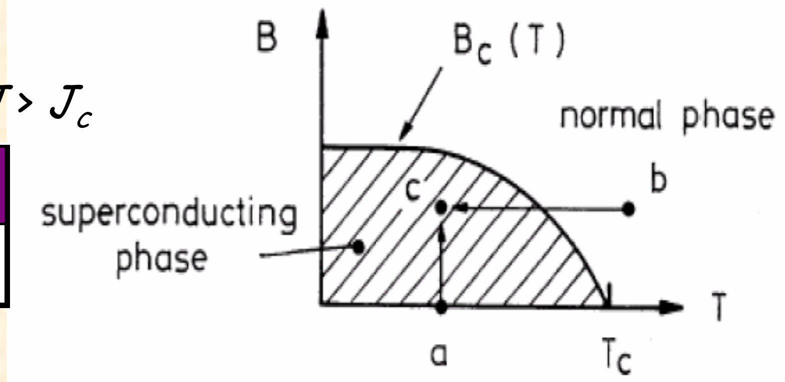
Below T_c the B-field lines are expelled out of a superconductor (perfect diamagnetic behaviour)



Type I superconductors

the superconductivity disappears as $T > T_c$ | $B > B_c$ | $J > J_c$

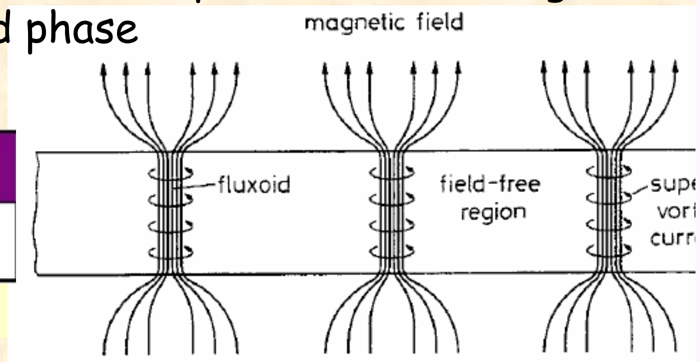
SC de type I	Ti	Al	Hg	Sn	Pb
B_c[mT] à 0 K	10	10,5	41,2	30,9	80,3

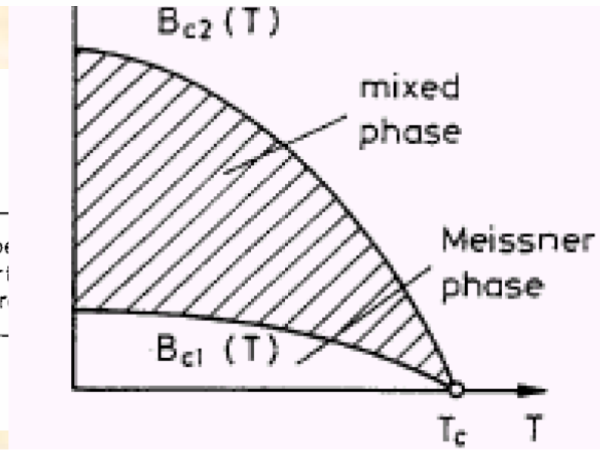


Type II superconductors

For $B_{c1} < B < B_{c2}$ there is a partial flux penetration through fluxoid vortexes and a mixed phase

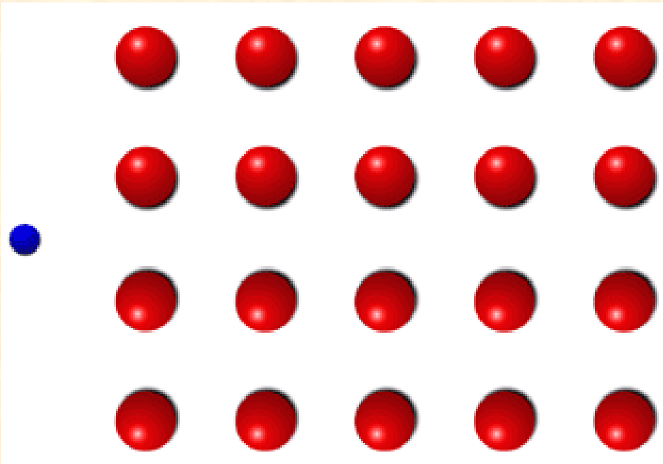
Nb (type II)	Bc_1	Bc_2
B_c[mT] à 0 K	~170	~240

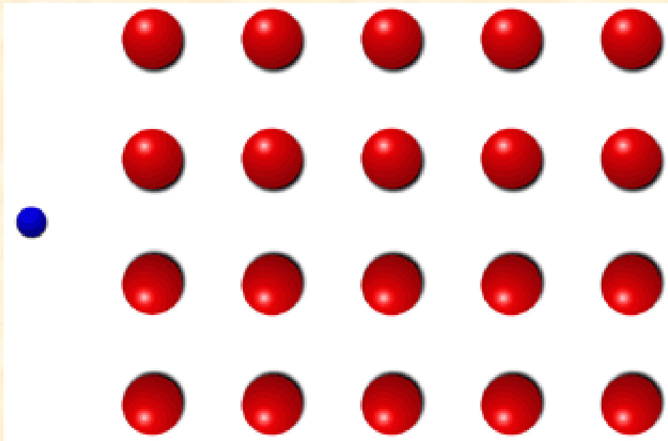




BCS Pairing mechanism

- **When electrons form pairs, they behave like bosons and can condensed into a macroscopic quantum state**
- **Bardeen, Cooper, and Shriffer (BCS) develop rigorous description of pairing mechanism**
  - **Theory developed in the 1950s, Nobel Prize in 1973**



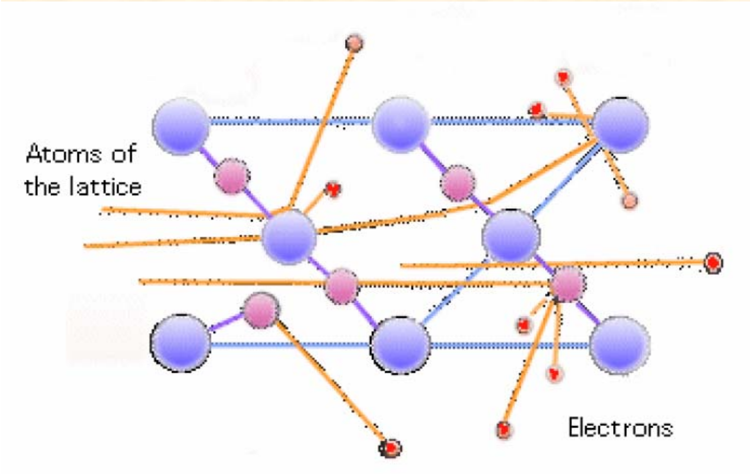


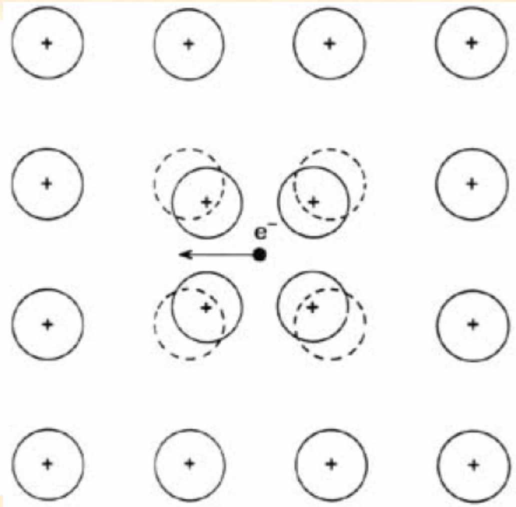
- **At T>20K, lattice vibration are strong and destroy pairs, superconductor becomes a normal metal**

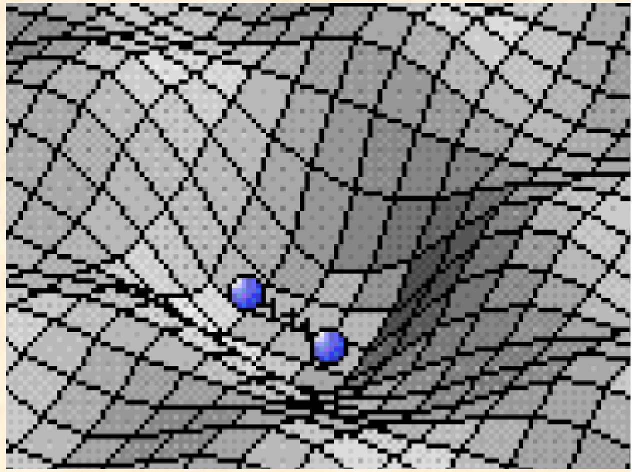
BCS theory

Normal conducting state

Superconducting state



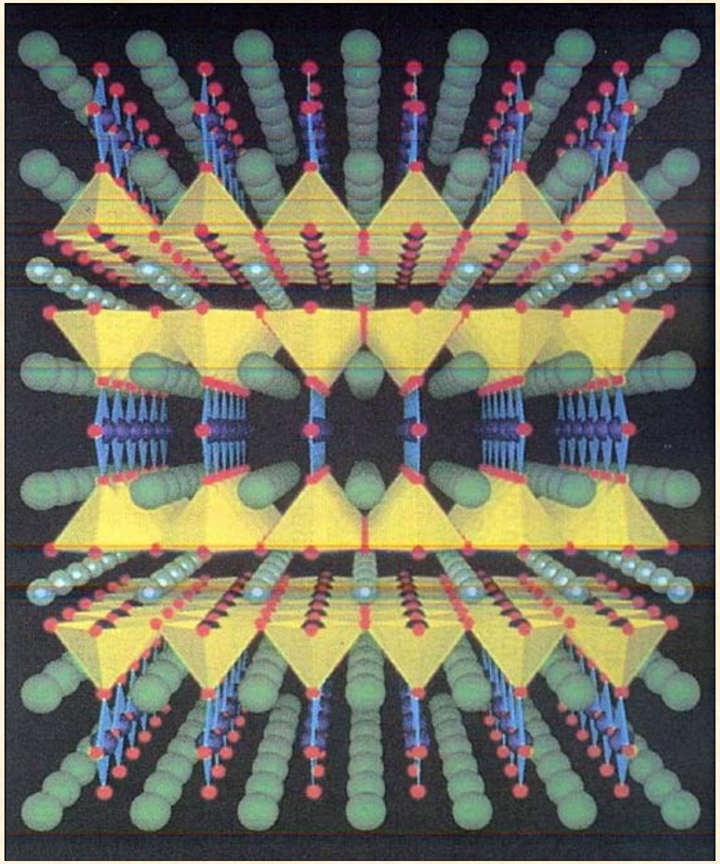




- $T_c \sim 1/\sqrt{M_{isotopic}}$ -> phonons should play a role in superconductivity
- Creation of Cooper pairs (over-screening effect)
  - An e^- attracts the surrounding ion creating a region of increased positive charge
  - The lattice oscillations enhance the attraction of another passing by e^- (Cooper pair)
  - The interaction is strengthened by the surrounding sphere of conduction e^- (Pauli principle)
- In a superconductor the net effect of e^-e^- attraction through phonon interaction and the e^-e^- coulombian repulsion is attractive and the Cooper pair becomes a singlet state with zero momentum and zero spin
- To break a pair the excitation energy is $\Delta E = 2\Delta$

High Temperature Superconductivity

- **Doped $YBa_2Cu_3O_7$**
  - **Normal states is insulating / poor metal**
  - **Discovered to be a SC with T_c=30K in 1986 (75 years after Kamerlingh-Onnes)**
  - **1987 Nobel Prize for Bednorz and Muller**
  - **Within years, other transition metal oxides were discovered with T_c>100K (liquid Nitrogen cooled SC)**
- **There is general agreement that the pairing mechanism is not phonon mediated**



Some examples of HTSC Compounds

- **Mostly compounds**
- **Record holder:**

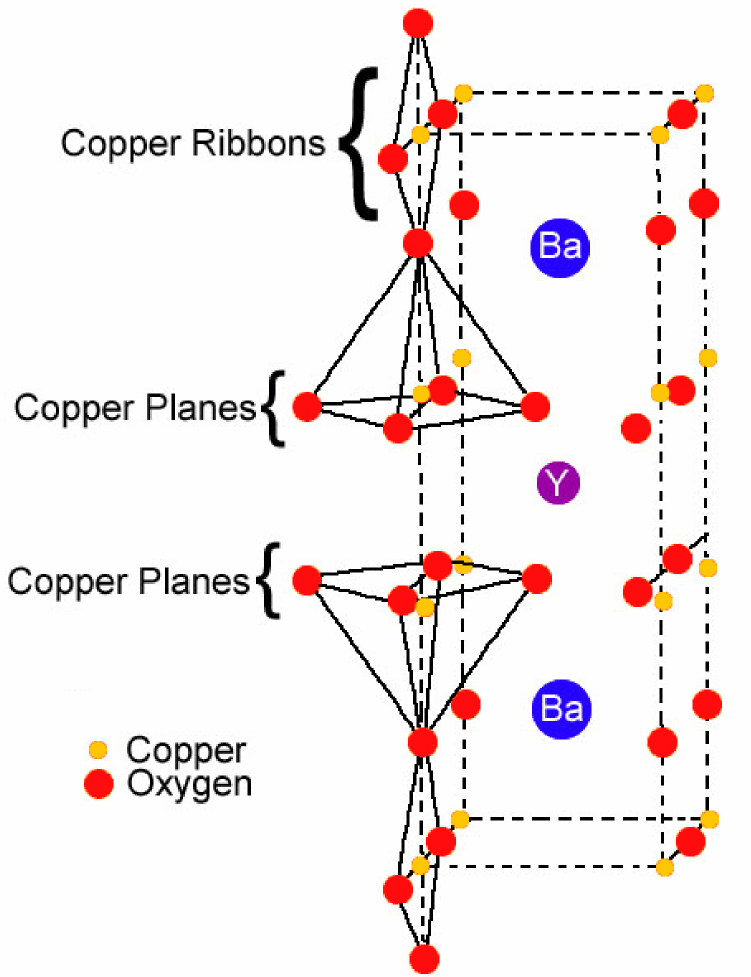
  Tc =138 K
- **High Hc2:**

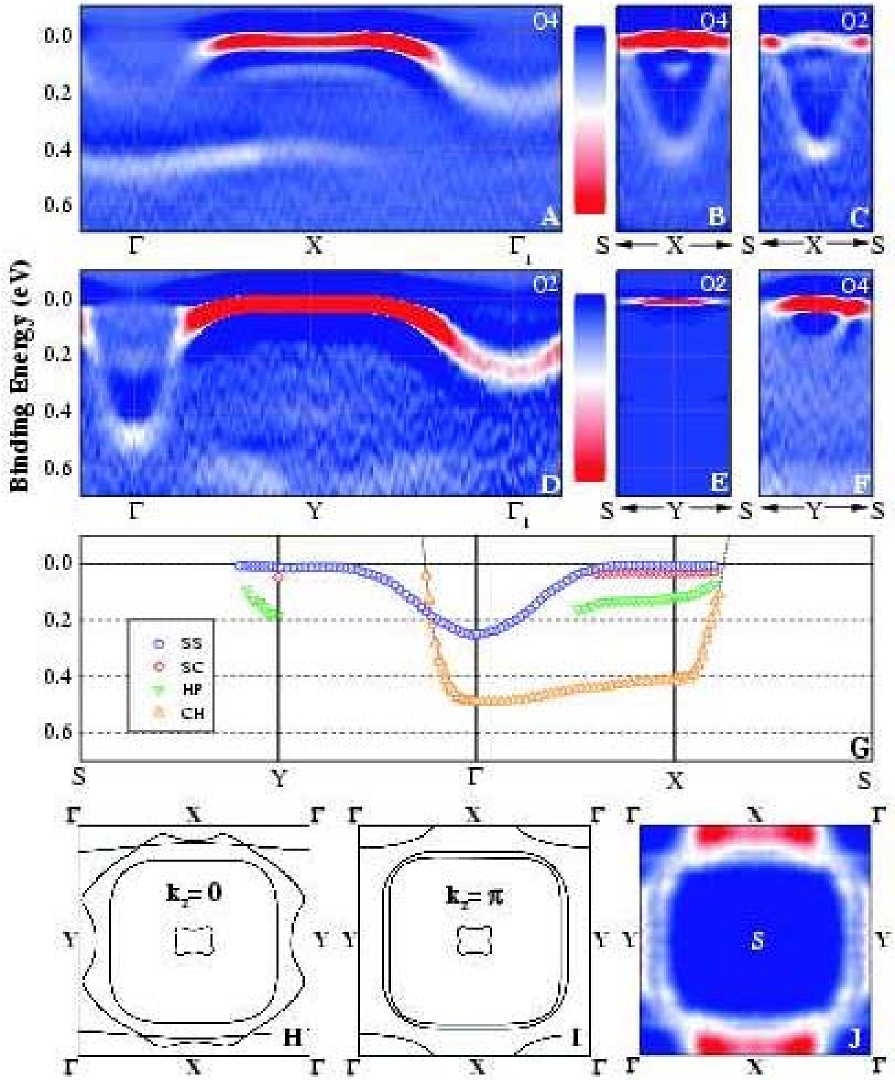
  Hc2 > 1000 000 G

  (YBCO)

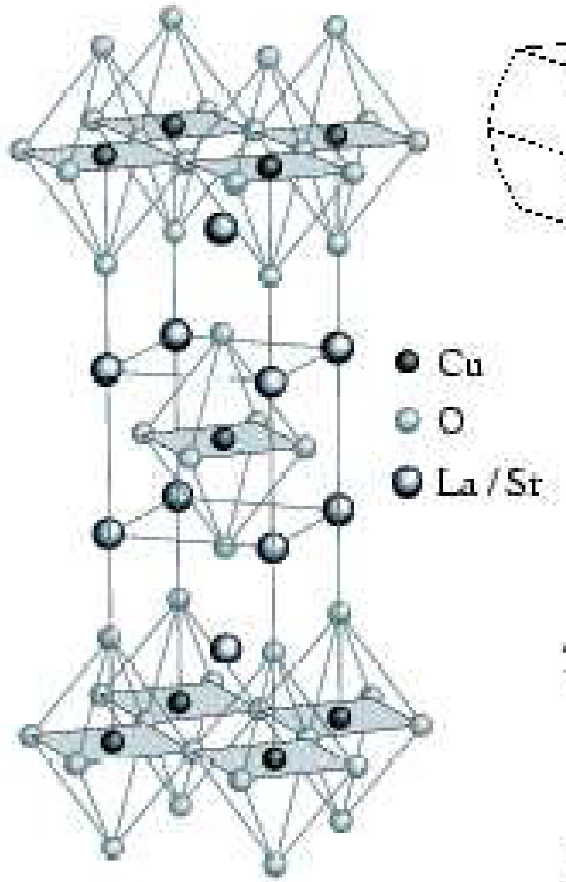
Element	Tc (K)
Tc	7.80
Nb	9.25
$La_{1.85}Ba_{.15}CuO_4$	30
$YBa_2Cu_3O_{7+}$	93
$Ca_{1-x}Sr_xCuO_2$	110
$Tl_2Ba_2Ca_2Cu_3O_{10}$	128
$Hg_{0.8}Tl_{0.2}Ba_2Ca_2Cu_3O_{8.33}$	138

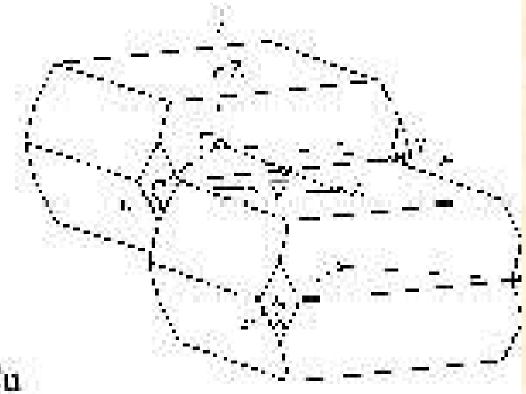
Crystal Structure and Fermi Surface

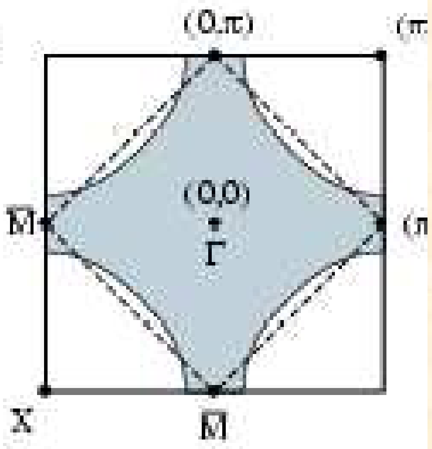


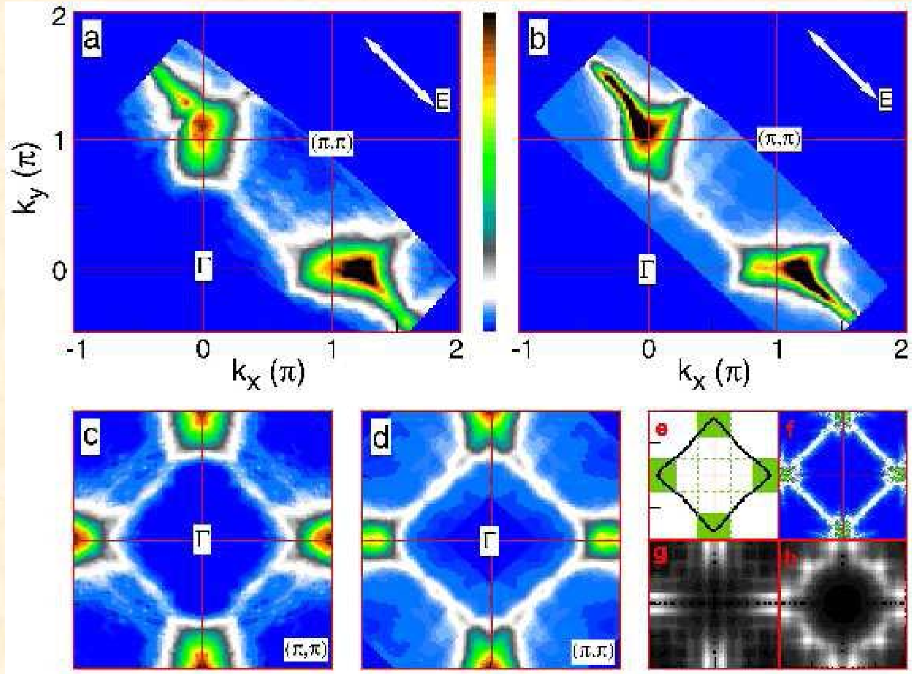


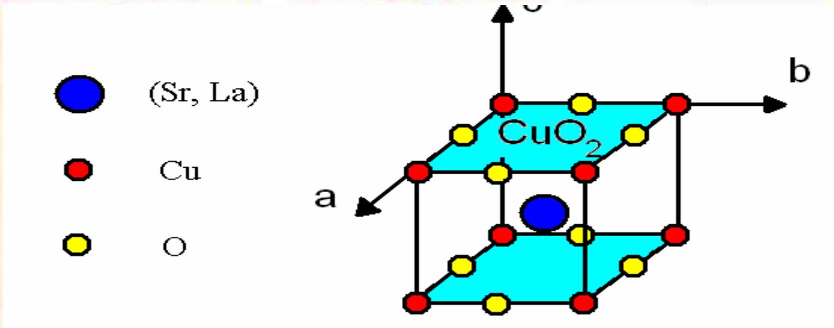
Crystal Structure and Fermi Surface



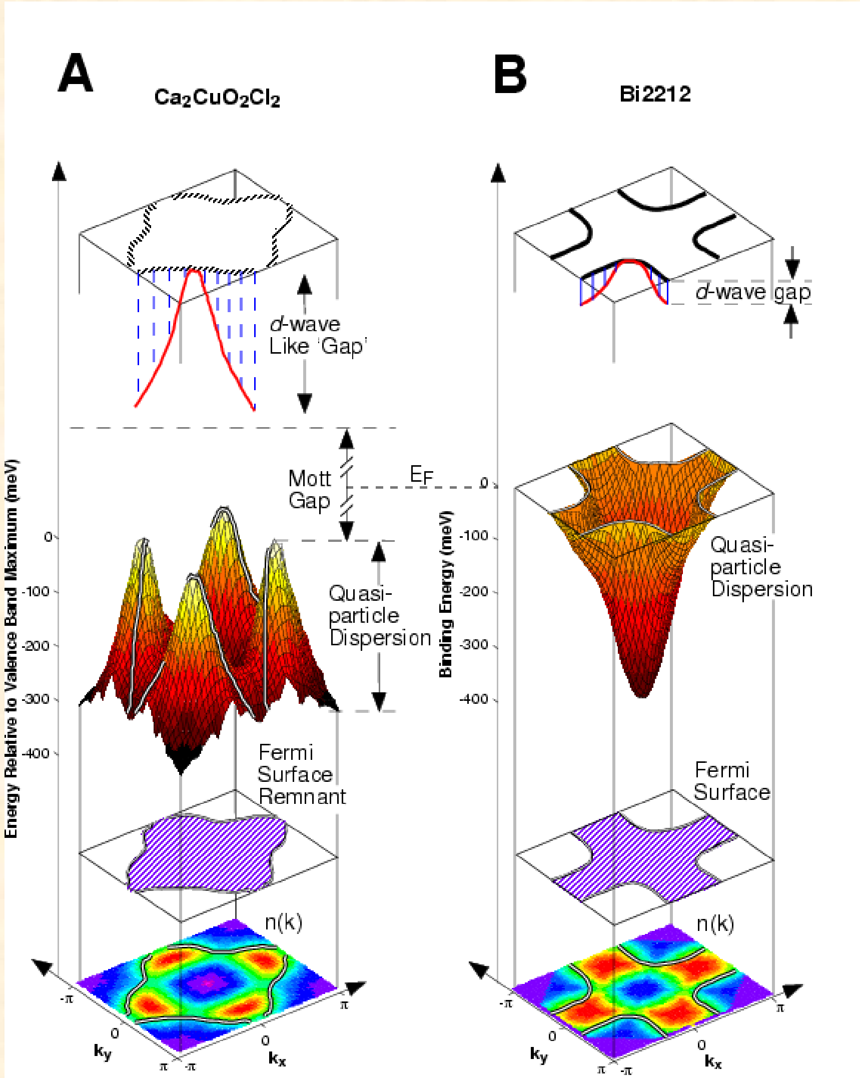






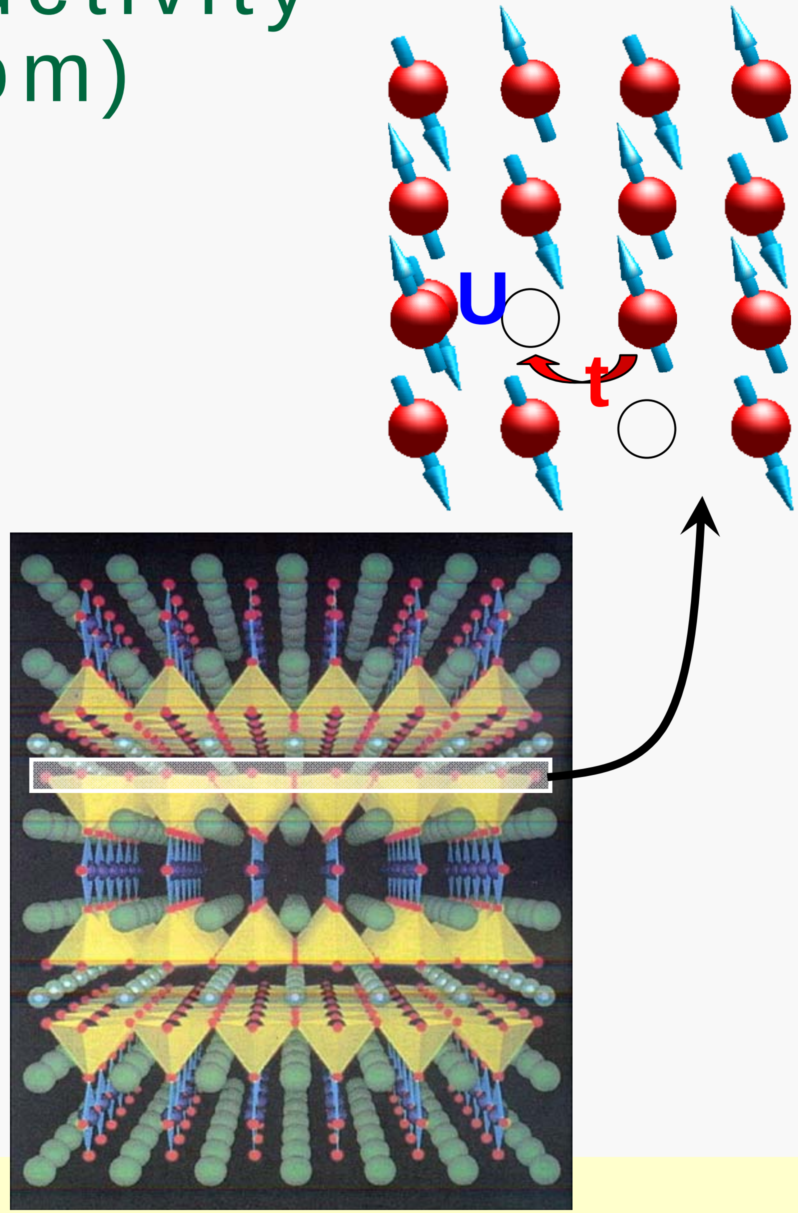


Crystal Structure and Fermi Surface

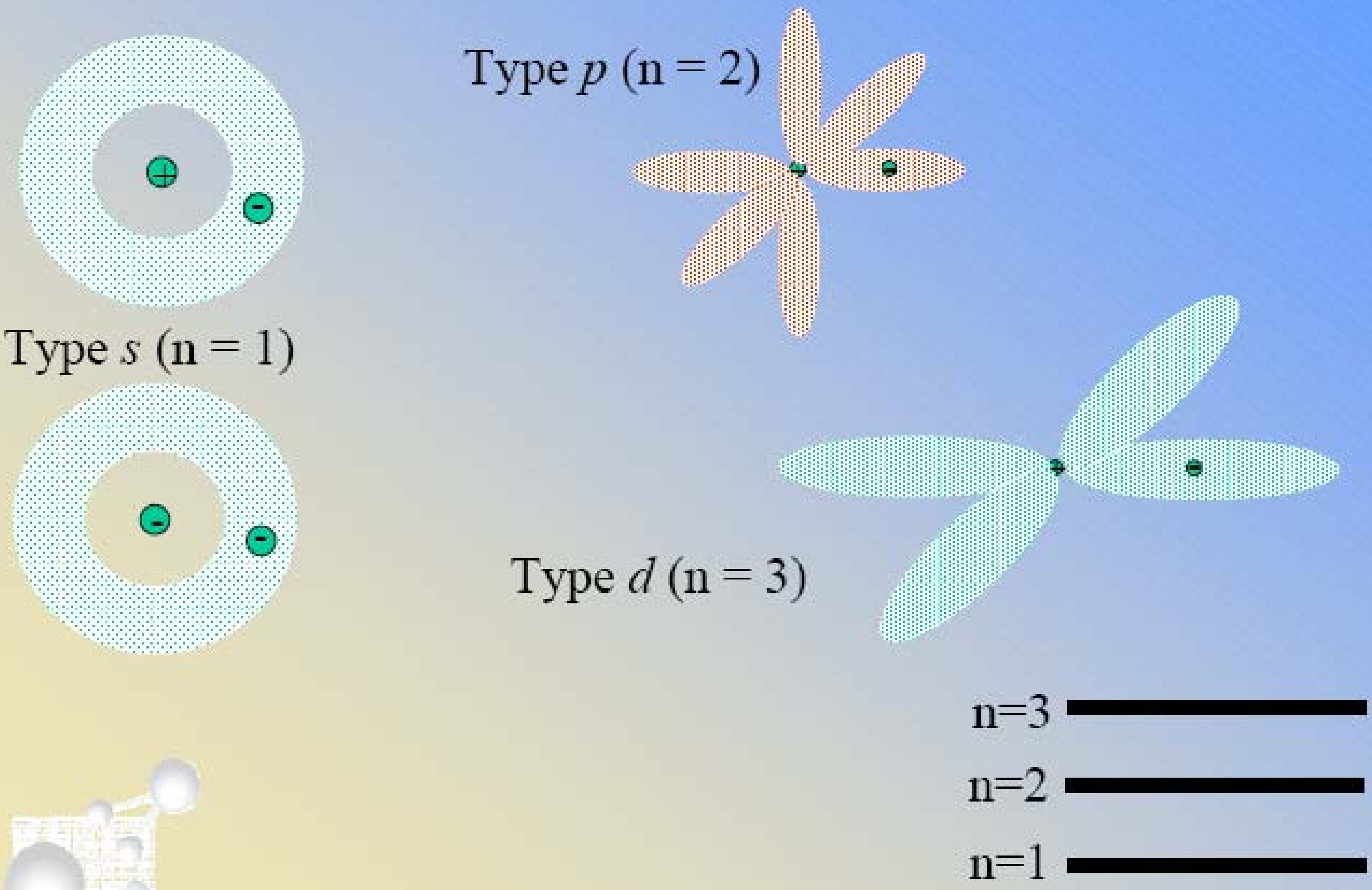


High Tc Superconductivity (conventional wisdom)

- **Model Copper oxide planes with single band 2D Hubbard models (Zhang & Rice, PRB 1989)**
- **Still not solvable, but thousands of papers published every year**
- **David Pines: “arguably the major problem in physics today”**



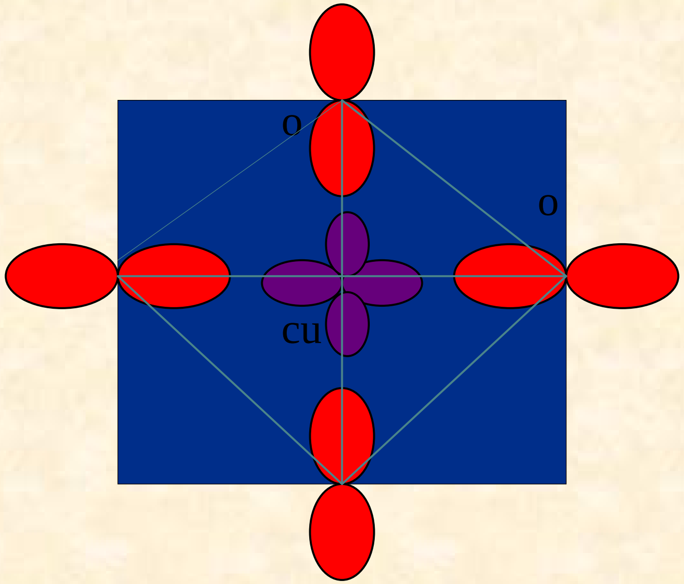
Understanding the mechanism --- Where are we ?



Microscopic Model:

Why are Cuprates Unique? (1987)

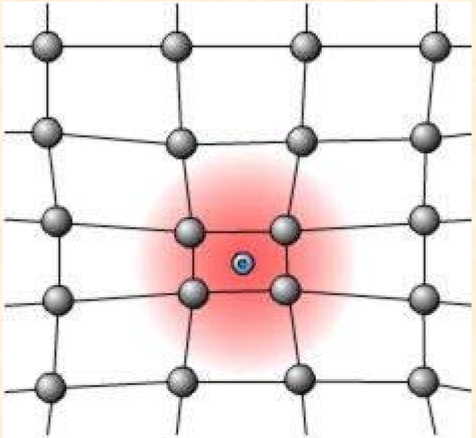
$Minimum\ Hamiltonian\ : Space\ of\ three\ orbitals\ (d, p_x, p_y)\ per\ unit\ cell:$
$\mathcal{H} = K.E.(t_{pd}, t_{pp}) + Local\ Repulsions\ (U_d, U_p) + \ Ionic\ Interactions\ (V).$

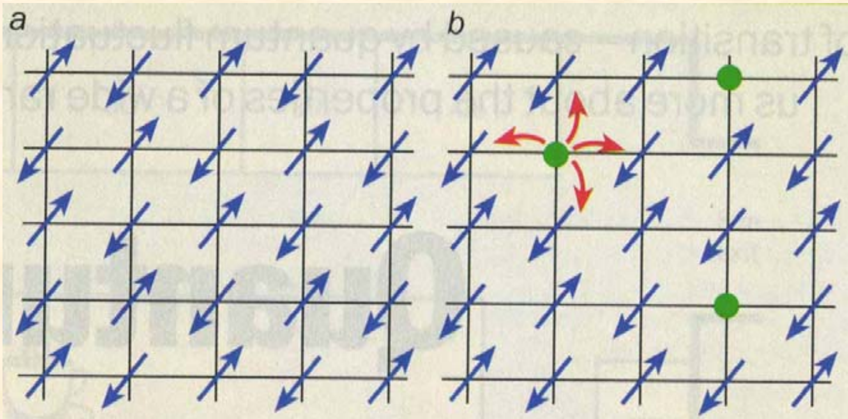


Cannot be reduced to a Hubbard Model because the ionization energy of Cu is nearly the same as the ionization energy of oxygen.

What interactions/orders exist in High-Tc Superconductor?

- **Electron-phonon interaction**



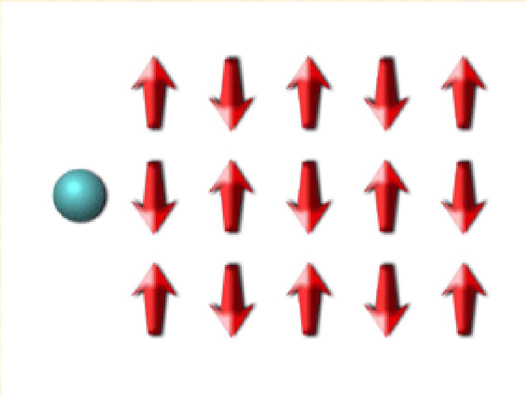


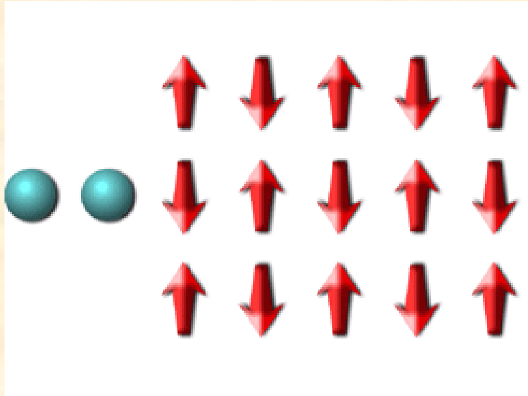
- **Spin exchange interaction-antiferromagnetic order**

- **Charge density waves, spin density waves and other competing orders.**

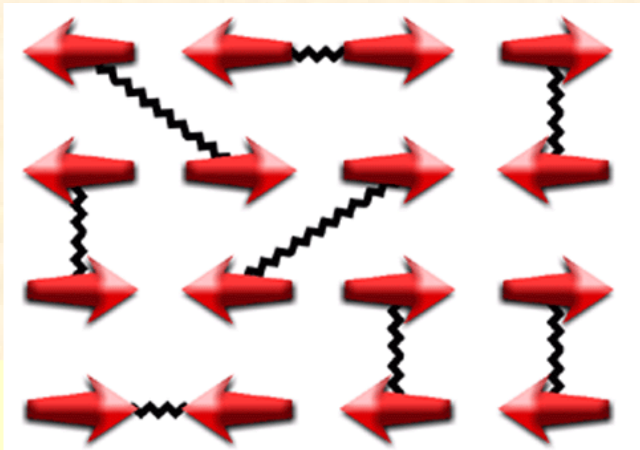
Of the many proposed pairing mechanisms, few remain likely:

- **Quasi particles in AF background (Hirsch 02)**

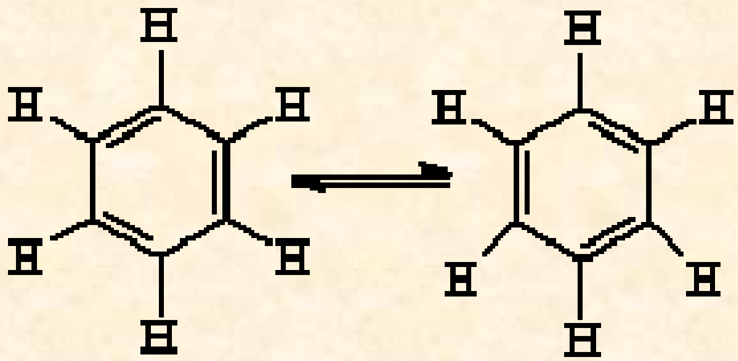


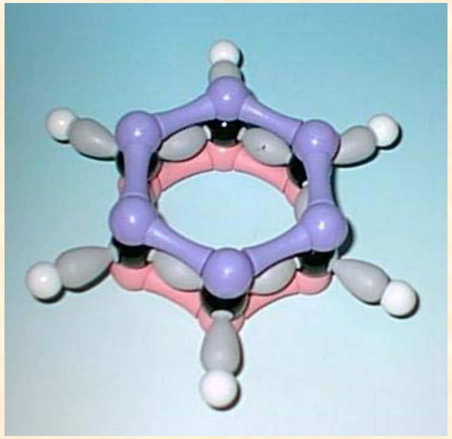


- **Resonating valence bond (Anderson 87)**



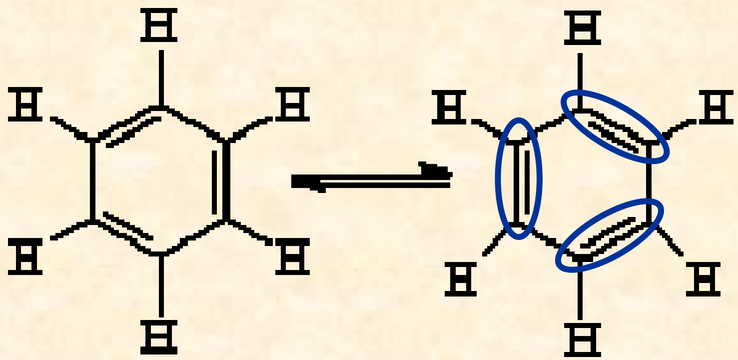
Valence bonds in benzene

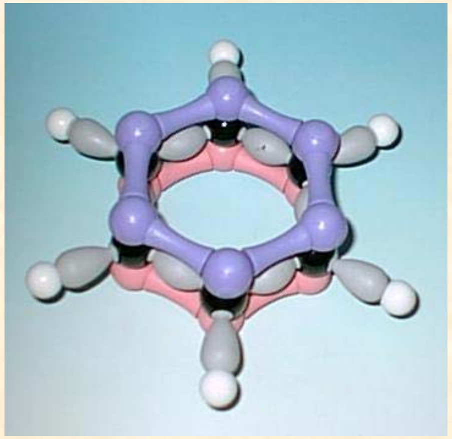




Resonance in benzene leads to a symmetric configuration of valence bonds
(*F. Kekulé, L. Pauling*)

Valence bonds in benzene





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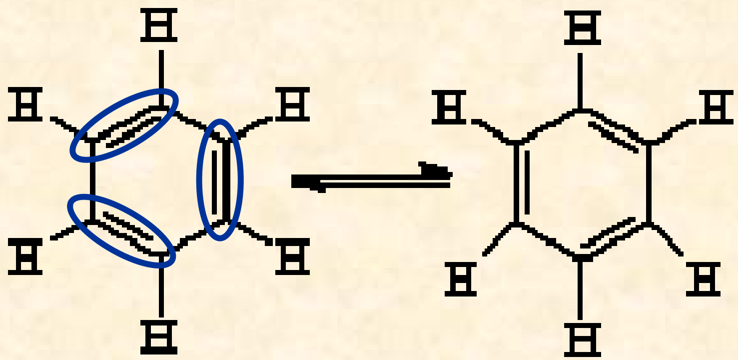

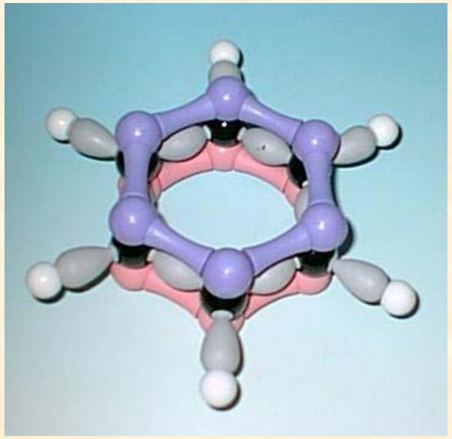

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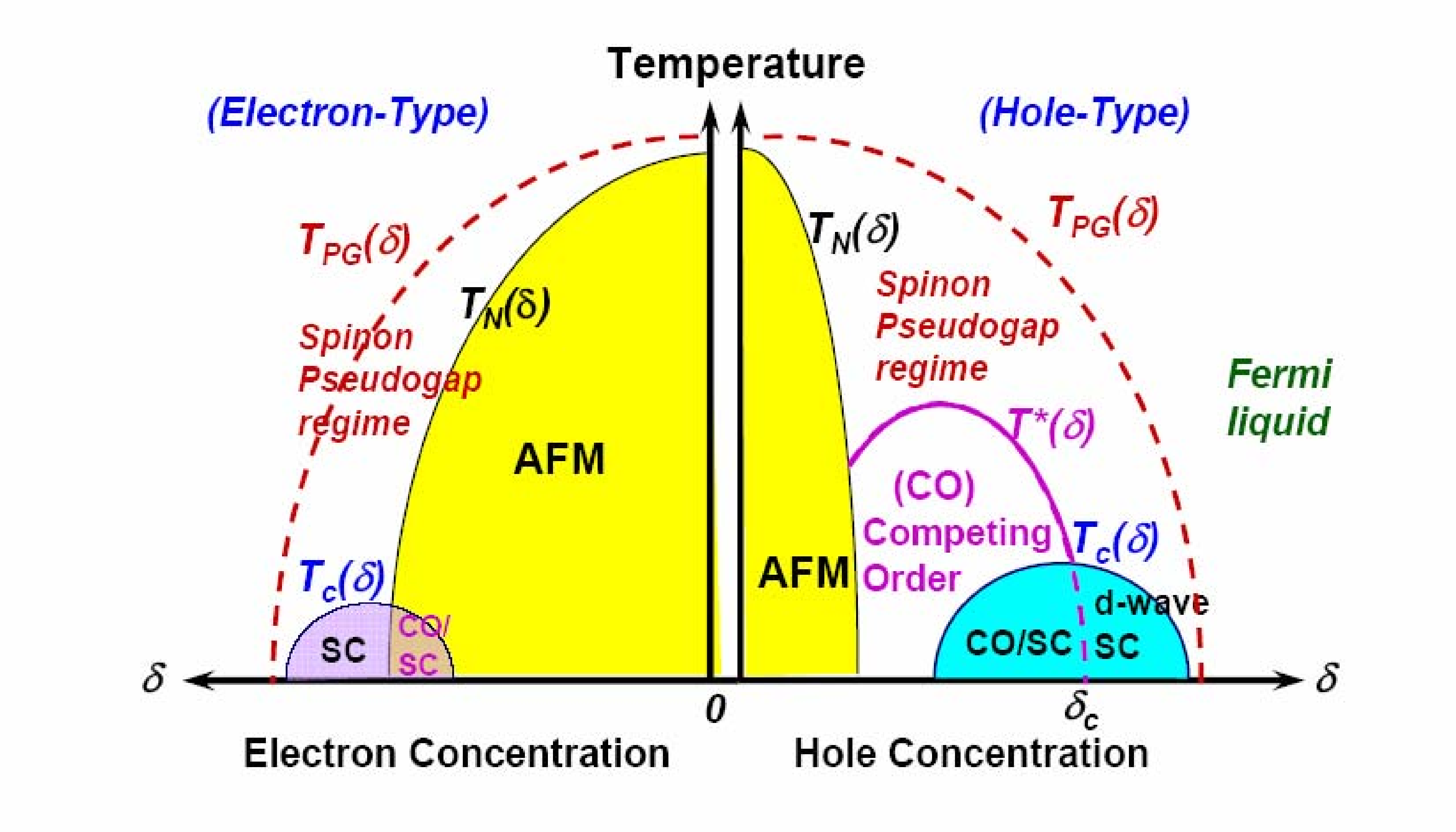
Phase Diagram and Competing Orders



PG: Pseudogap, SC: Superconductivity, CO: Competing order, AFM: Antiferromagnetic

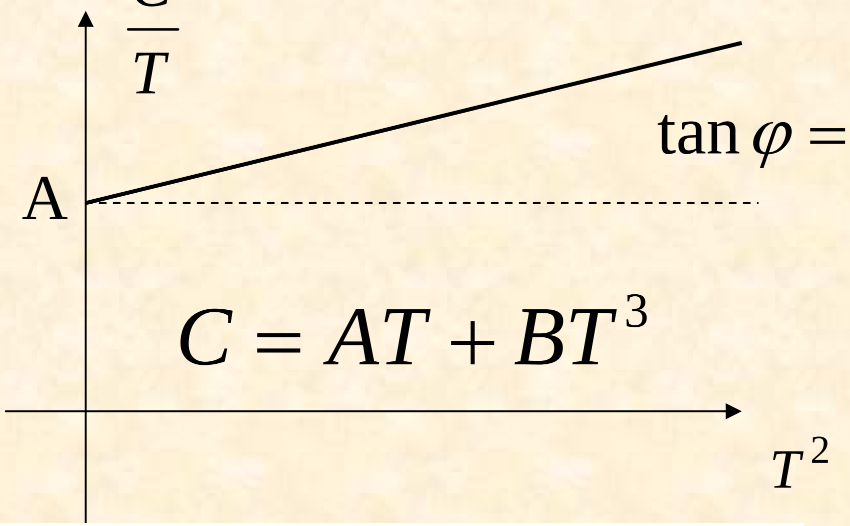
Strongly Correlated Systems:

Heavy Fermions

Heavy Fermions

Type	Material	T^*	$T_c,\ x_c,\ B_c$	Properties	ρ	γ_n $mJmol^{-1}K^{-2}$	Ref.
Metal	$CeCu_6$	$10K$	-	Simple HF Metal	T^2	1600	[1]
Super-conductors	$CeCu_2Si_2$	$20K$	T_c=0.17K	First HFSC	T^2	800-1250	[2]
	UBe_{13}	2.5K	T_c=0.86K	Incoherent metal→HFSC	$\rho_c \sim$ 150$\mu\Omega$cm	800	[3]
	$CeCoIn_5$	38K	T_c=2.3K	Quasi 2D HFSC	T	750	[4]
Kondo Insulators	$Ce_3Pt_4Bi_3$	$T_\chi \sim 80K$	-	Fully Gapped KI	$\sim e^{\Delta/T}$	-	[5]
	$CeNiSn$	$T_\chi \sim 20K$	-	Nodal KI	Poor Metal	-	[6]
Quantum Critical	$CeCu_{6-x}Au_x$	$T_0 \sim 10K$	$x_c = 0.1$	Chemically tuned QCP	T	$\sim \frac{1}{T_0} \ln\left(\frac{T_0}{T}\right)$	[7]
	$YbRh_2Si_2$	$T_0 \sim 24K$	$B_\perp$=0.06T $B_\parallel$=0.66T	Field-tuned QCP	T	$\sim \frac{1}{T_0} \ln\left(\frac{T_0}{T}\right)$	[8]
SC + other Order	UPd_2Al_3	110K	T_{AF}=14K, T_{sc}=2K	AFM + HFSC	T^2	210	[9]
	URu_2Si_2	75K	T_1=17.5K, T_{sc}=1.3K	Hidden Order & HFSC	T^2	120/65	[10]

Specific heat



$$C = AT + BT^3$$

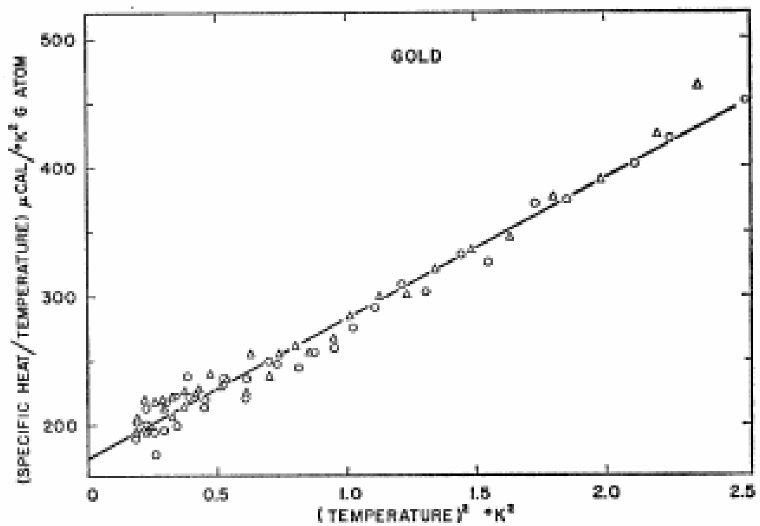


FIG. 1. Plot of (specific heat/temperature) versus (temperature²) for gold.

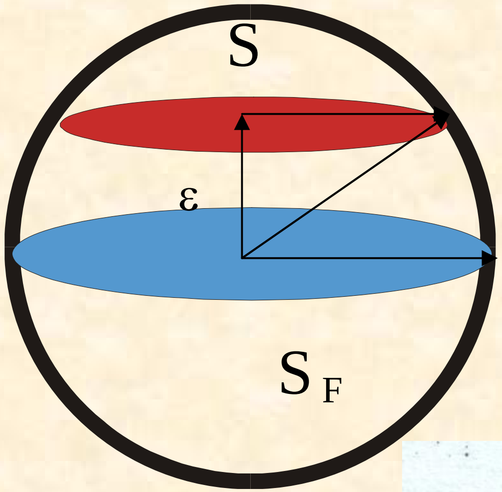
$$E = 2V \int \epsilon(p) n(\epsilon_p) \frac{d^3p}{(2\pi\hbar)^3}$$

$$C = V^{-1}\left(\frac{\partial E}{\partial T}\right)_V = 2\int \epsilon(p)\left(\frac{\partial n(\epsilon_p)}{\partial T}\right)\frac{d^3p}{(2\pi\hbar)^3}$$

$$C = \frac{\pi^2}{3}\rho(0)T = \gamma T \qquad \gamma = \frac{p_F m^*}{3\hbar^3} \qquad \rho(0) = \frac{p_F m^*}{\pi^2\hbar^3}$$

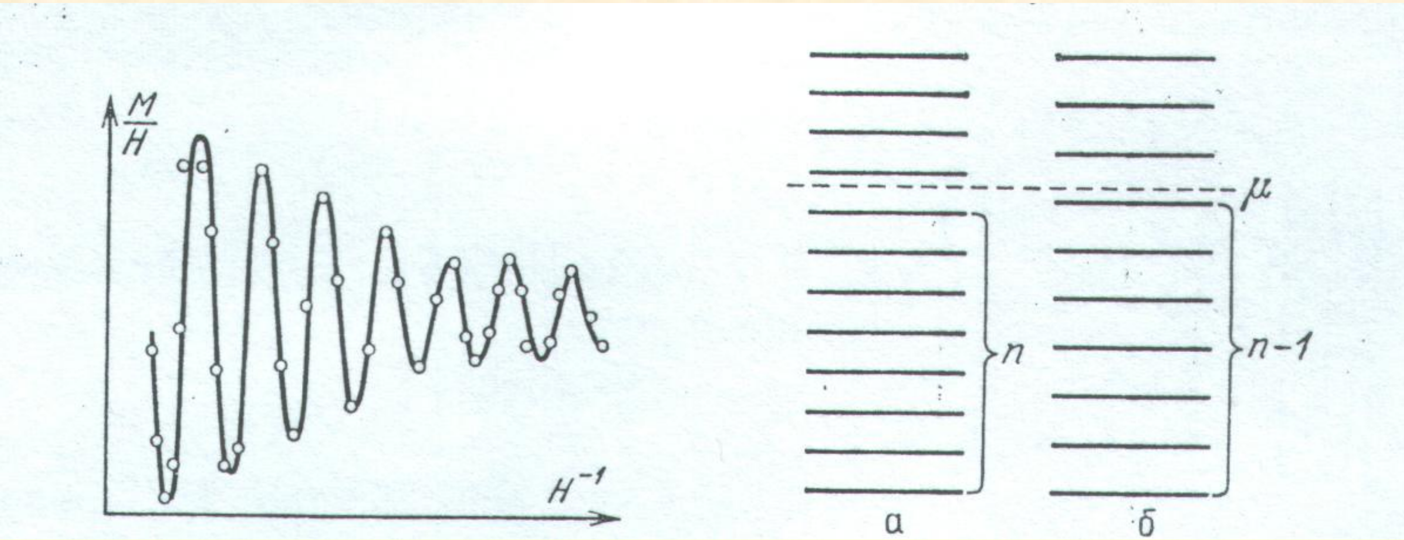
	N/V $[cm^{-3}]$	ϵ_F [eV]	T_F [K]	m^*/m
Li	4.6×10^{22}	4.7	5.5×10^4	2.3
Na	2.5	3.1	3.7	1.3
K	1.34	2.1	2.4	1.2
Cu	8.5	7.0	8.2	1.3
Ag	5.76	5.5	6.4	1.1
Au	5.9	5.5	6.4	1.1

de Haas-van Alphen Effect (dHvA)

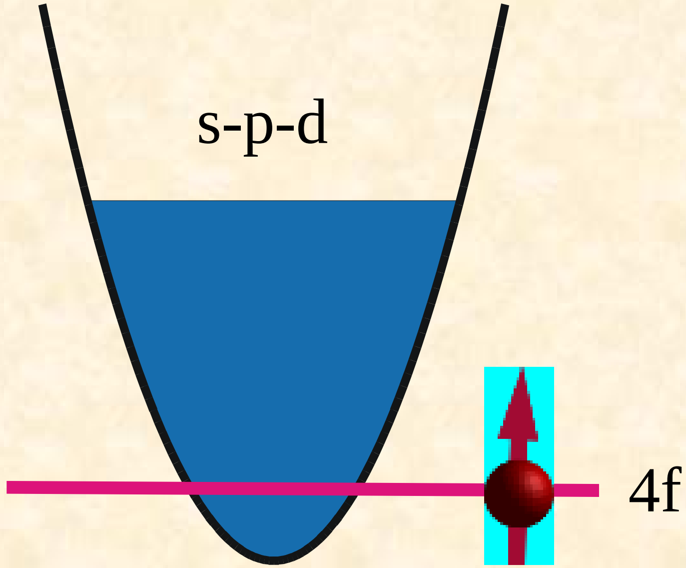


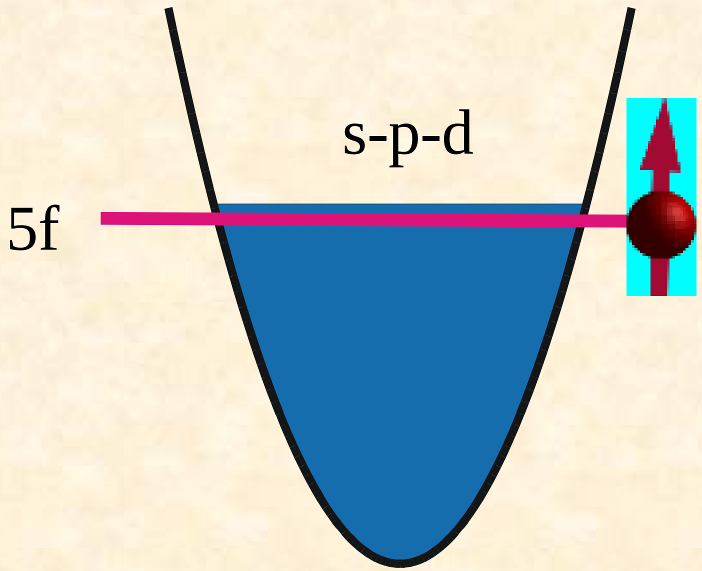
$$M \approx T\sqrt{\frac{2e\hbar}{\pi^3 cH}}\sum_m S_m \left|\frac{\partial^2 S_m}{\partial p_z^2}\right| \exp\left(-\frac{2\pi^2 T c m^*}{e\hbar H}\right)\sin\left(\frac{cS_m}{e\hbar H}\pm\frac{\pi}{4}\right)\cos\left(\frac{\pi m^*}{m}\right)$$

$$m^* = \frac{1}{2\pi}\frac{\partial S}{\partial \epsilon}$$

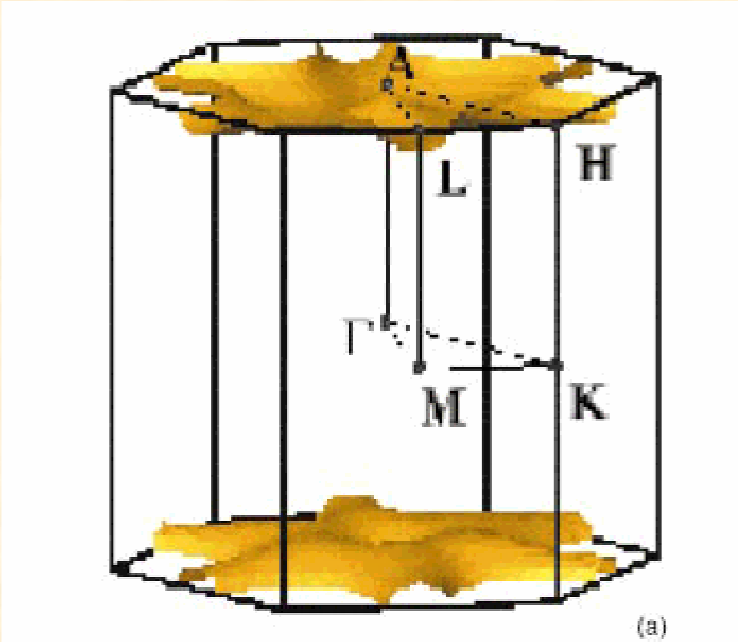


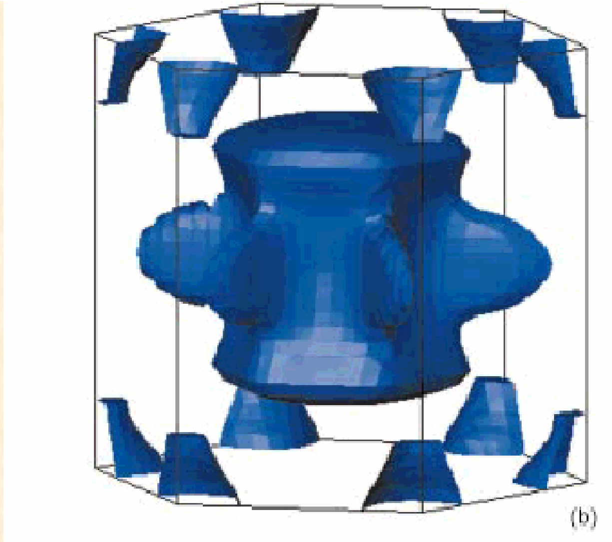
Heavy Fermion Compounds

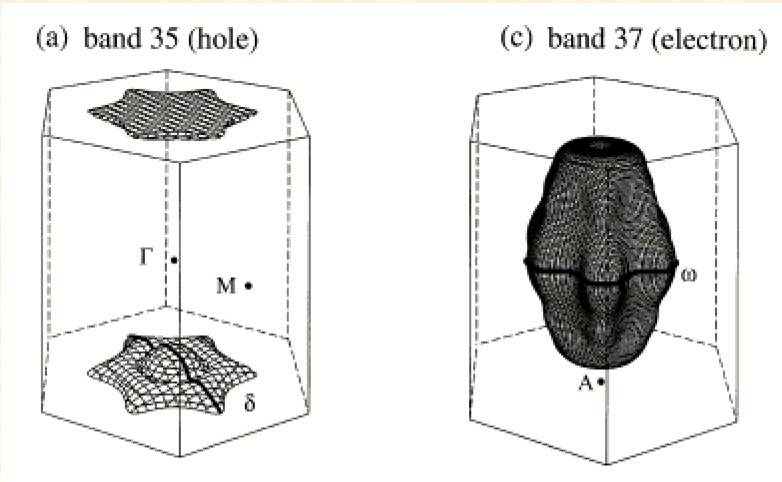


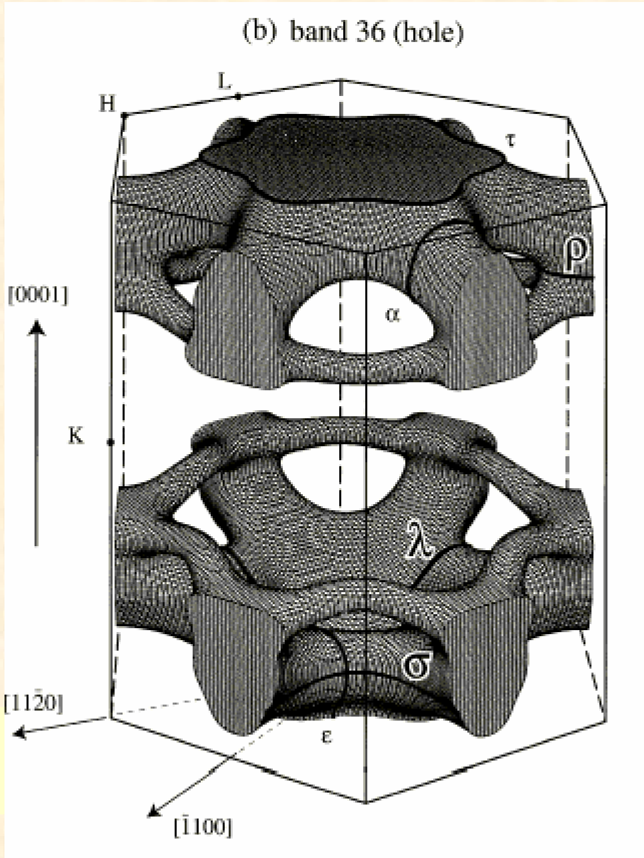


System	γ_0 (J/K^2mol)	T_F K	m^*/m	T_c K	T_K K
$CeCu_6$	1.6	300	500	-	5
$CeAl_2$	0.14	4000	42	-	3.9
$CeCu_2Si_2$	1.1	350	450	0.8	10
$CeRu_2Si_2$	0.35	1200	100	-	20
UBe_{13}	0.72	700	260	-	8
UPt_3	0.42	1100	180	5	80
UCd_{11}	1.42	400	425	5	-
U_2Zn_{17}	0.42	1100	180	10	-


A
L
H
Γ
M
K
(a)


(b)


(a) band 35 (hole)
(c) band 37 (electron)
Γ
M
δ
ω
A


(b) band 36 (hole)
H
L
τ
ρ
[0001]
α
K
λ
σ
[11$\bar{2}$0]
ε
[$\bar{1}$100]

Models: Kondo Lattice

$$H = \sum_k \varepsilon(k) c^+_{k,\sigma} c_{k,\sigma} + J \sum_i \vec{S}_i \vec{s}_i + \sum_{ij} I_{ij} \vec{S}_i \vec{S}_j$$

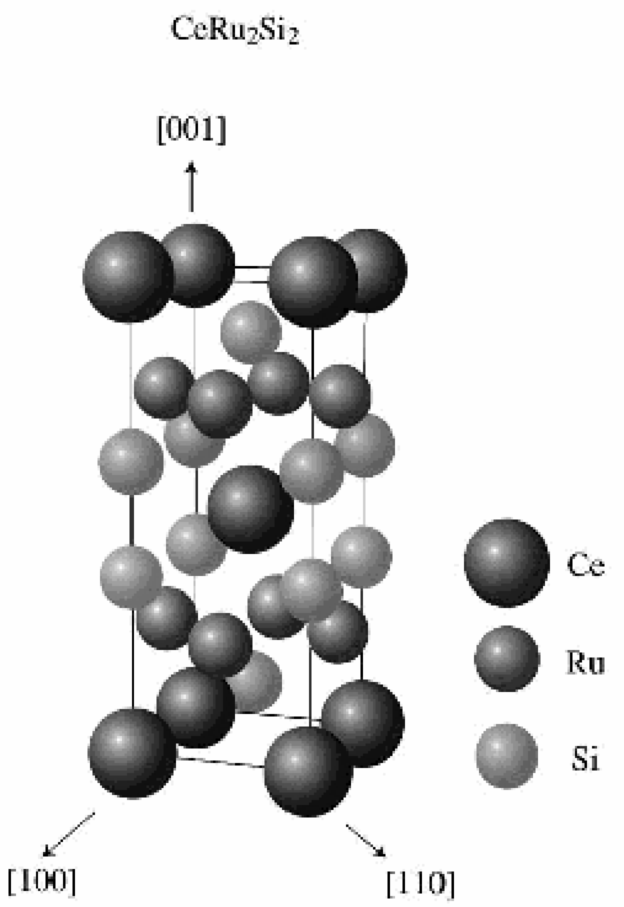
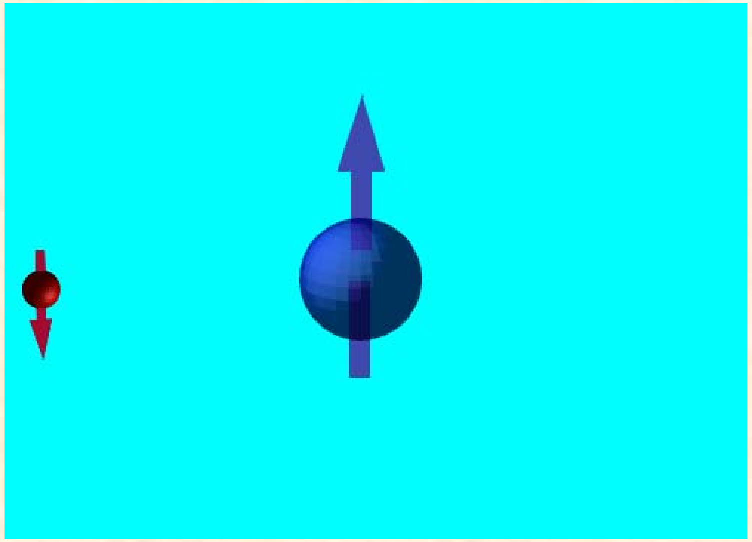


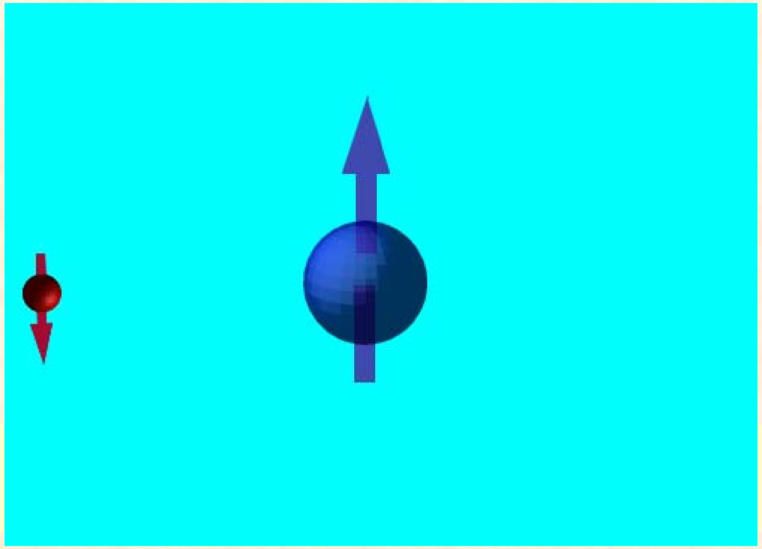
Fig. 10. Crystal structure of $CeRu_2Si_2$.

$$H_{Kondo} = J \sum_i \vec{S}_i \vec{s}_i$$

$$H_{RKKY} = \sum_{i,j} I_{ij} \vec{S}_i \vec{S}_j$$

Kondo-Effect

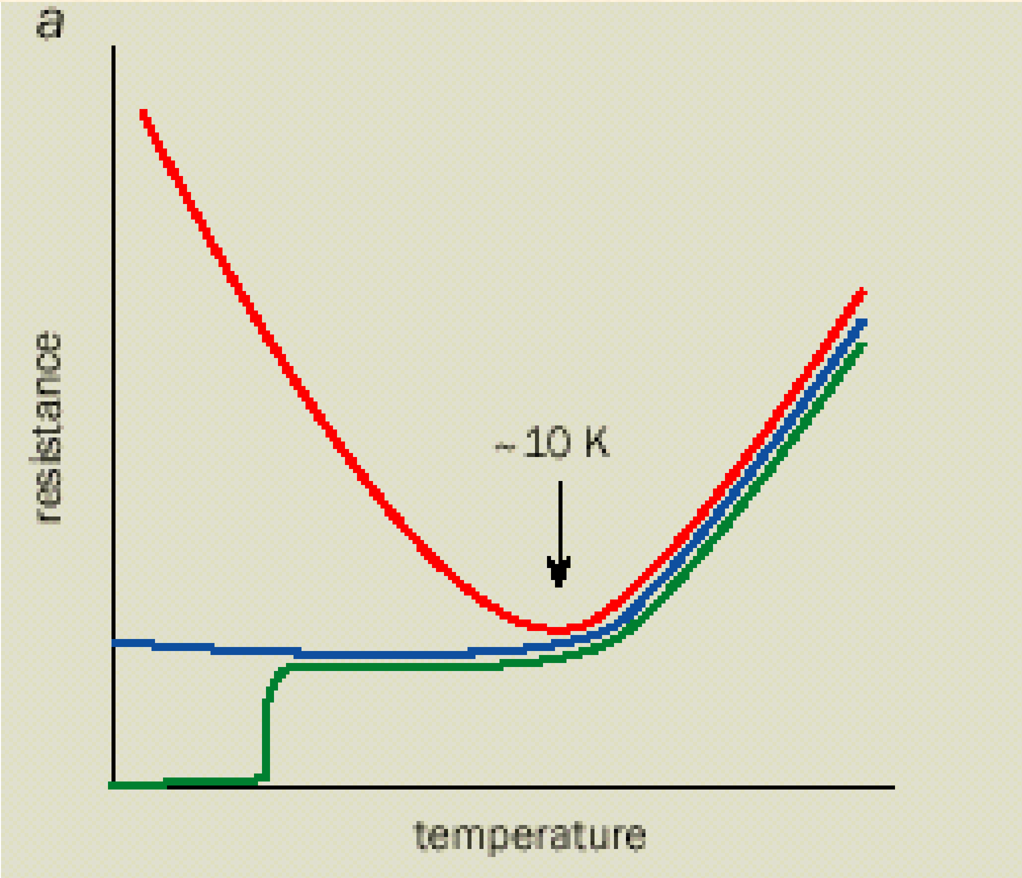




$$H_{Kondo} = J\sum_i \vec{S}_i \vec{s}_i$$

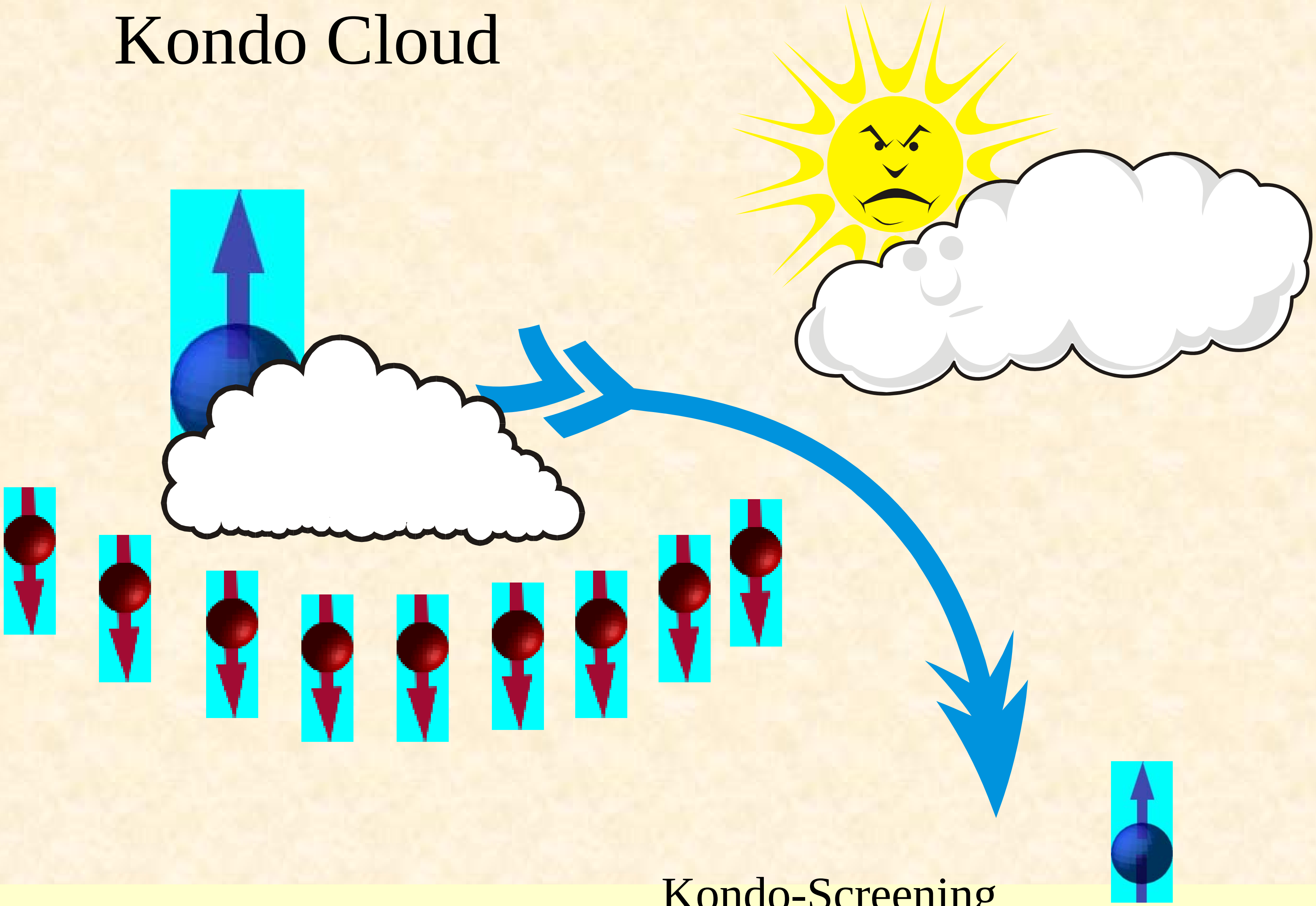
$$\rho = \rho_v + c_m a \ln(\mu/T) + bT^5$$

Resistance at low temperatures



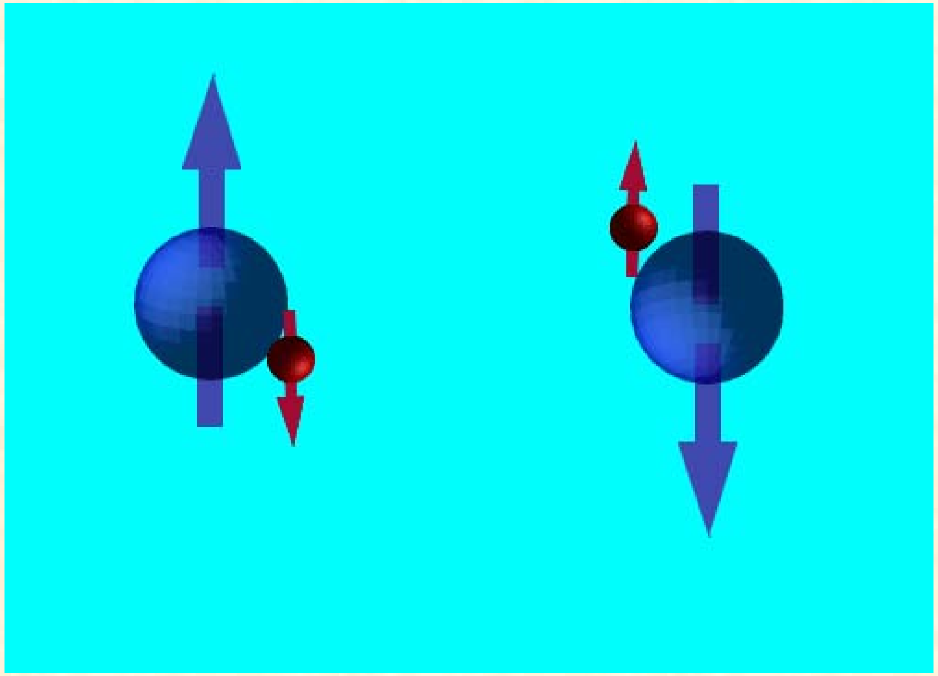
$$\rho = \rho_v + c_m a \ln(\mu/T) + bT^5$$

Kondo Cloud

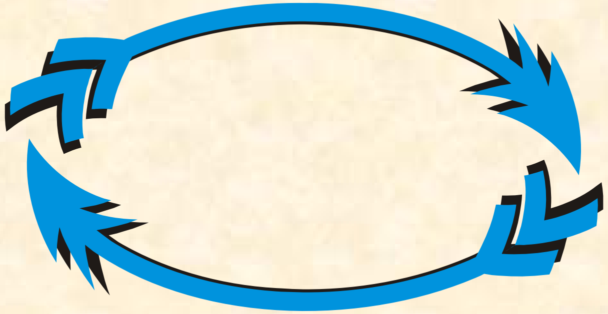


Kondo-Screening

Ruderman-Kittel-Kasuya-Yosida (RKKY) Wechselwirkung

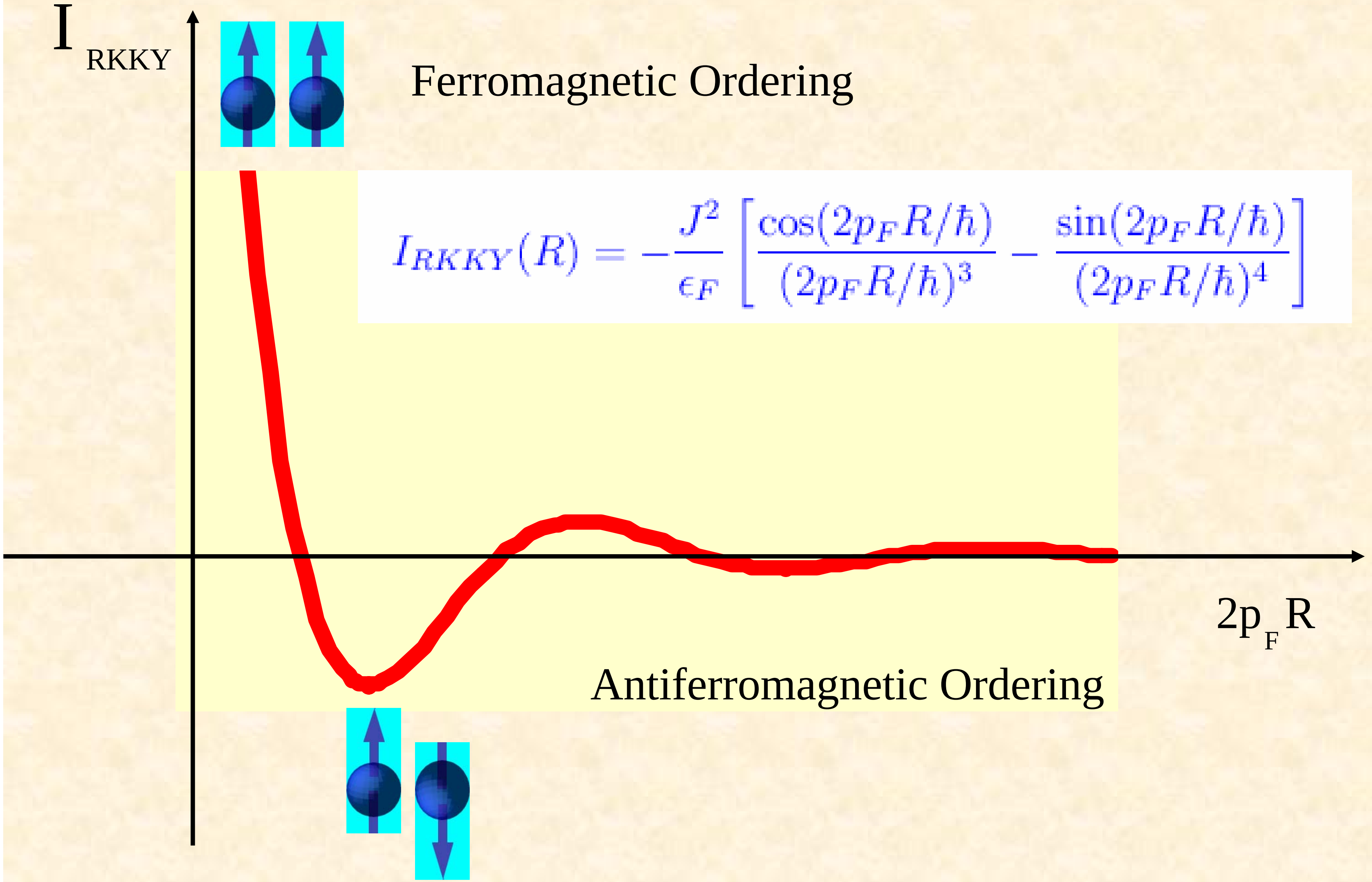


$$H_{RKKY} = \sum_{i,j} I_{ij} \vec{S}_i \vec{S}_j$$



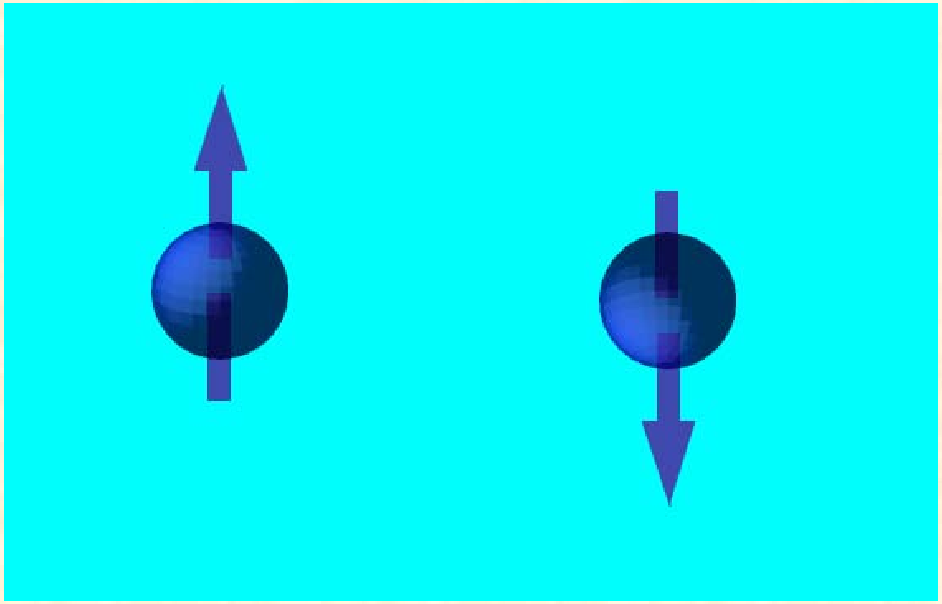
$$I_{RKKY} = 2\left(\frac{J}{n}\right)^2 \sum_{p,p'} \frac{n_{\mathbf{p}}(1-n_{\mathbf{p}'})}{\epsilon_{\mathbf{p}} - \epsilon_{\mathbf{p}'}}$$

$$I_{RKKY}(q) = -\frac{m^* p_F}{4\pi^2\hbar^3}\left(\frac{J}{n}\right)^2 \left[1 + \frac{(2p_F)^2 - q^2}{4p_F q} \ln\left|\frac{2p_F - q}{2p_F + q}\right|\right]$$



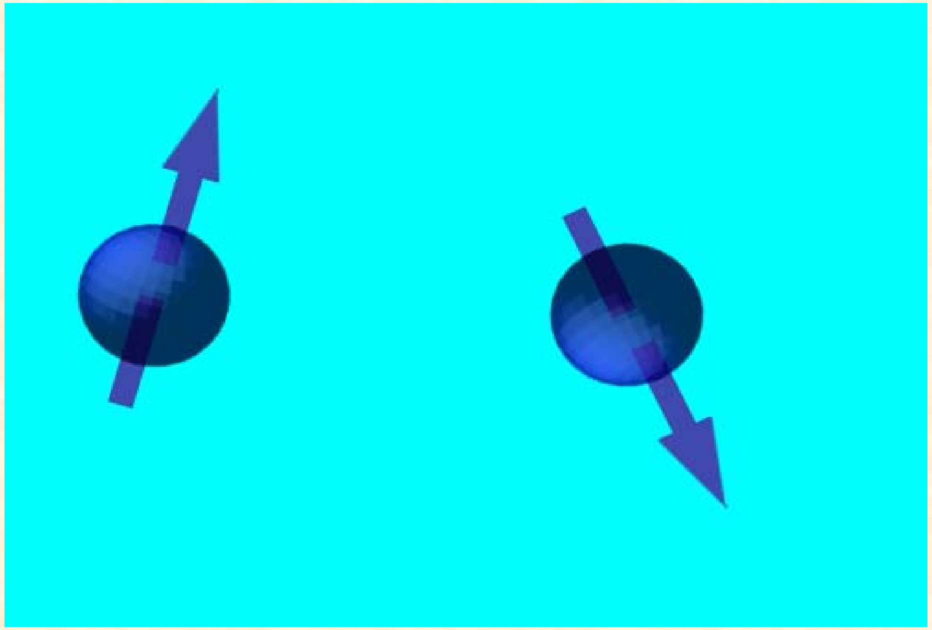
$$I_{RKKY}(R) = -\frac{J^2}{\epsilon_F}\left[\frac{\cos(2p_F R/\hbar)}{(2p_F R/\hbar)^3} - \frac{\sin(2p_F R/\hbar)}{(2p_F R/\hbar)^4}\right]$$

Antiferromagnetic Ordering



$$T > T_c$$

$$\mathcal{N} = \tanh\left(\frac{I_{\mathbf{Q}}\mathcal{N}}{2T}\right)$$

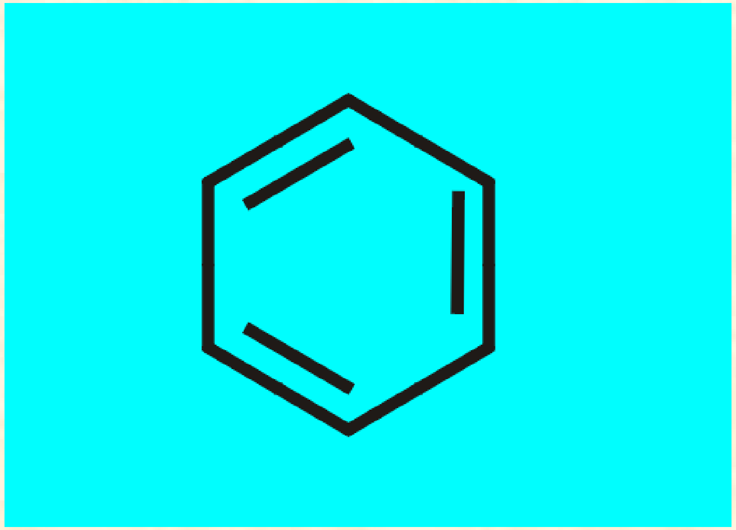


$$T < T_c$$

$$\mathcal{N} = \tanh\left(\frac{I_{\mathbf{Q}}\mathcal{N}}{2T}\right)\left[1 - \frac{a_N}{\ln(T/T_K)}\frac{\cosh^2(\beta I_{\mathbf{Q}}\mathcal{N}/2)}{\cosh^2(\beta I_{\mathbf{Q}}\mathcal{N})}\right]$$

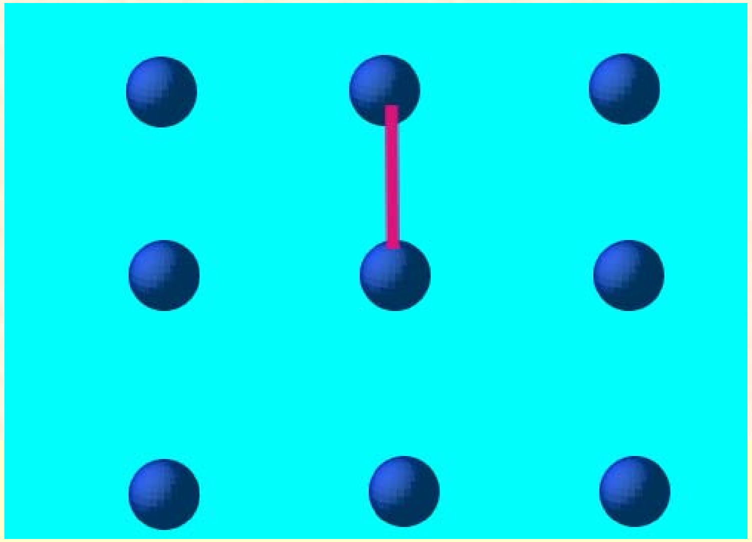
Spin Liquid

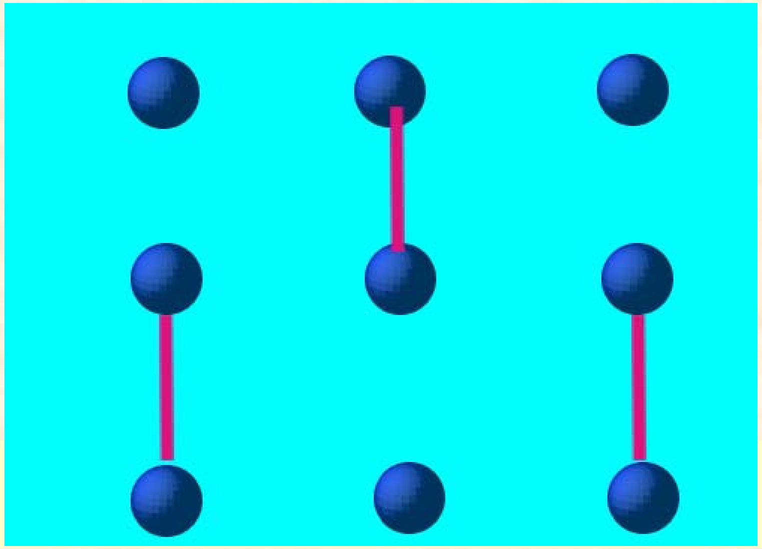
Resonating Valence Bonds



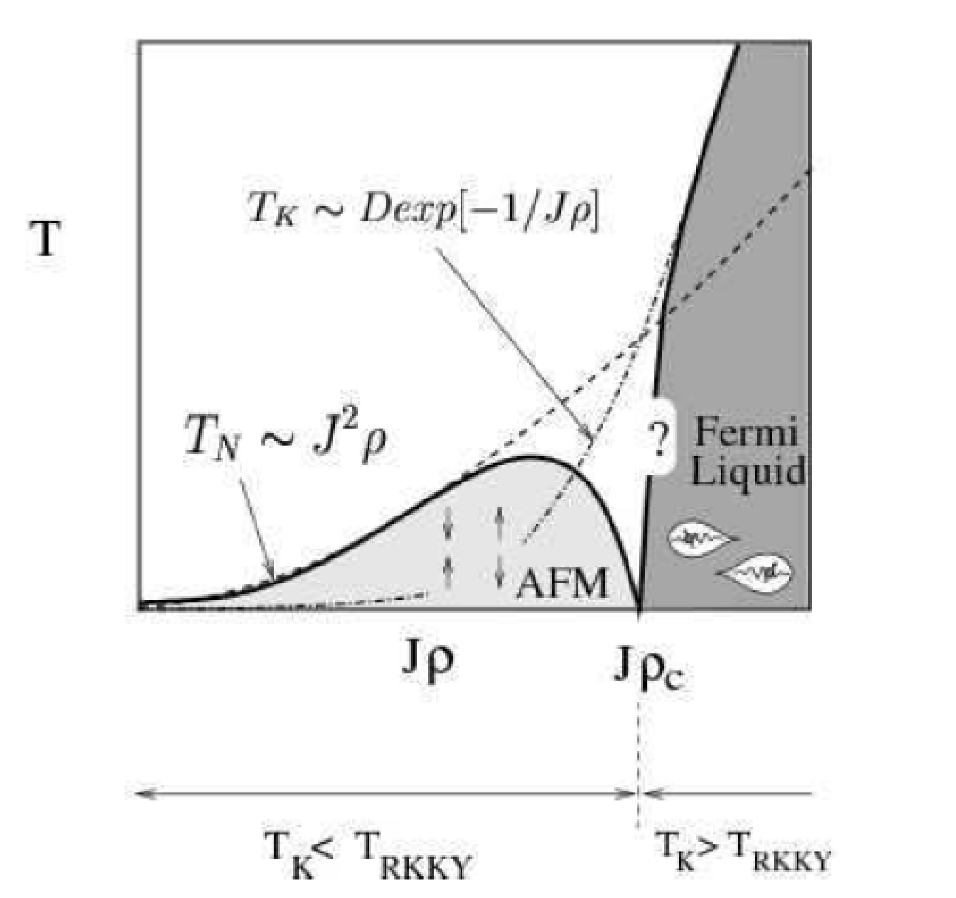
$$\Delta = -\sum_{\mathbf{q}} \nu(\mathbf{q}) \tanh\left(\frac{I_{\mathbf{q}}\Delta}{T}\right)$$

$$\Delta = -\sum_{\mathbf{q}} \nu(\mathbf{q}) \left[\tanh\left(\frac{I(\mathbf{q})\Delta}{T}\right) + a_{sl}\frac{I_{\mathbf{q}}\Delta}{T\ln(T/T_K)}\right]$$





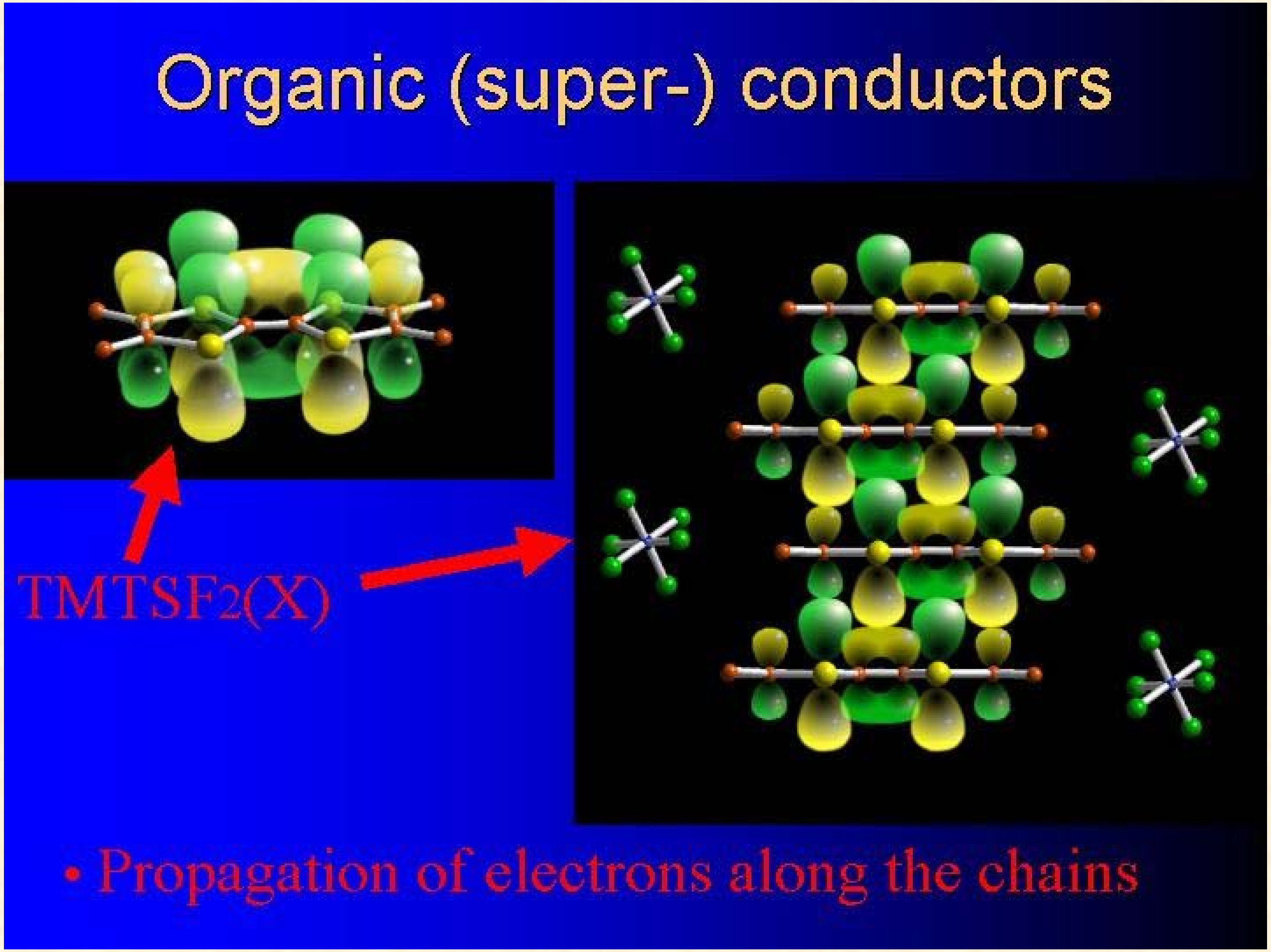
Heavy Fermions: Phase Diagram

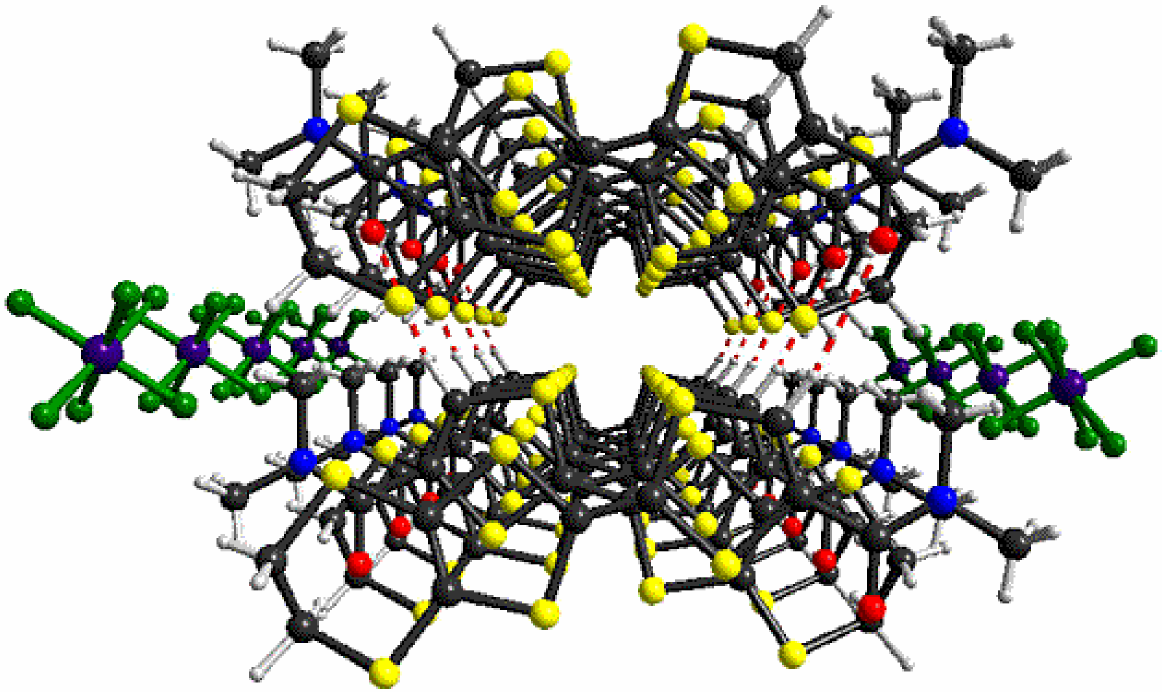


Strongly Correlated Systems:

Organic Conductors

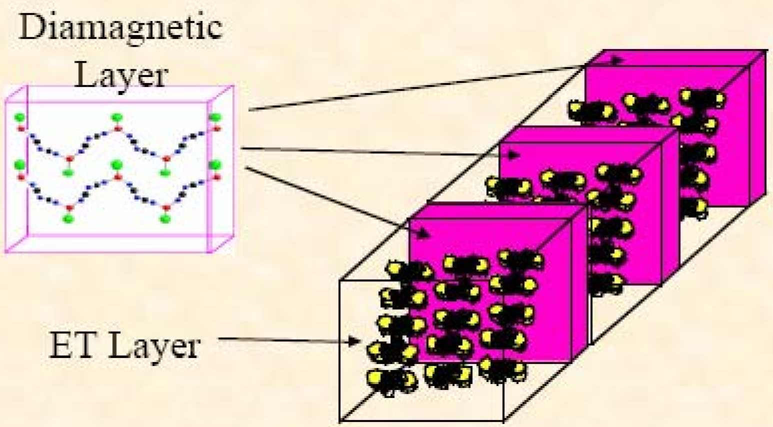
Bechgaard salts

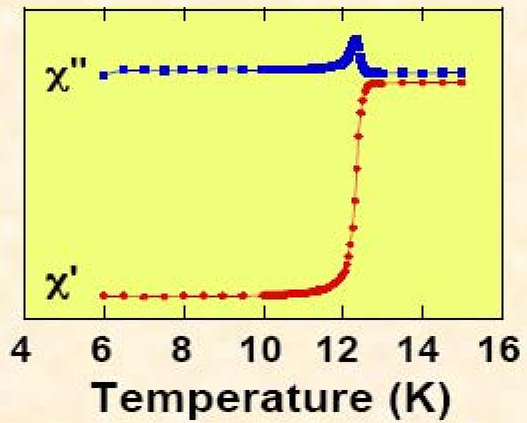




A perspective down the criss-cross stacks in $[EDT\text{-}TTF\text{-}CONMe_2]_2AsF_6$

Molecular Superconductors



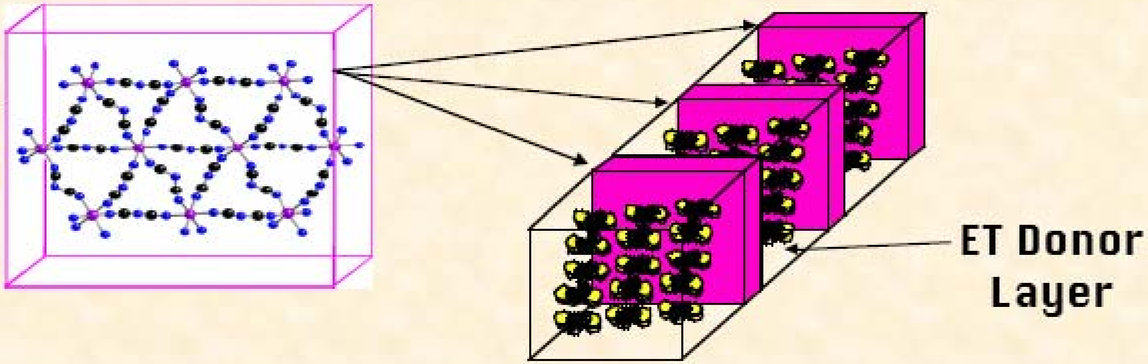


ET=BEDT-TTF

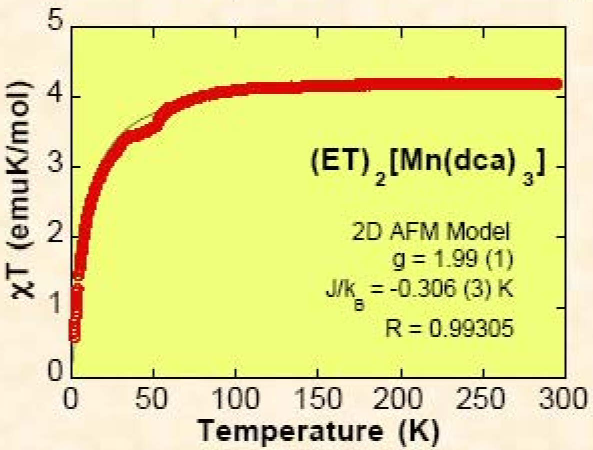
Bis(EthyleneDiThio) TetraThiaFulvalene

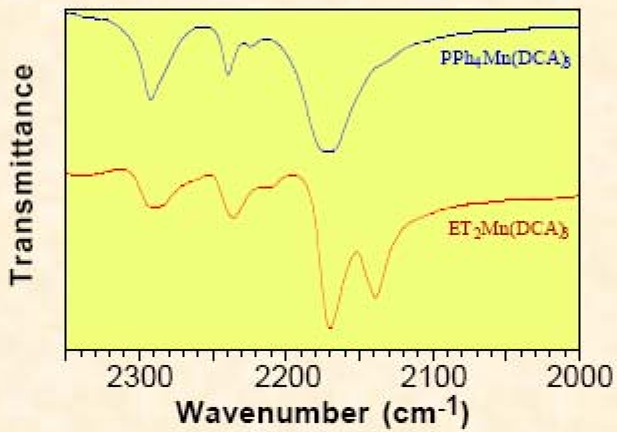
J.A.Schlueter et al, 2004

Conducting/Magnetic Hybrid Molecular Solids



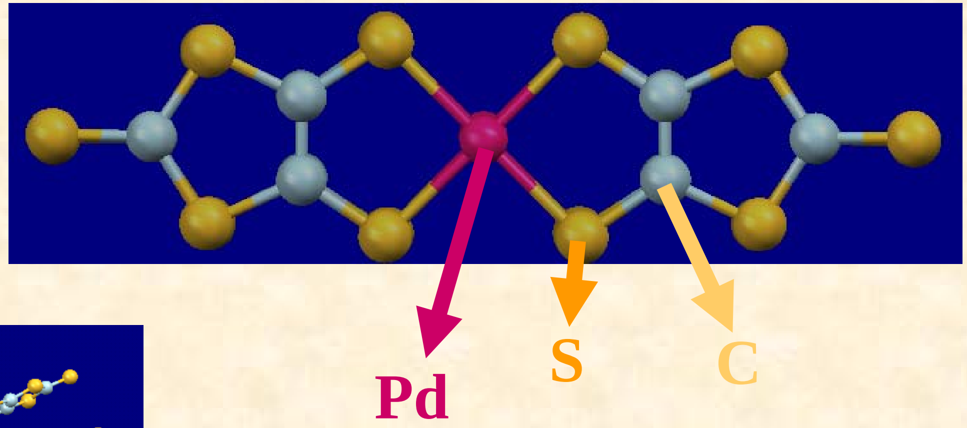
Incorporation of magnetic layer between ET donor layers

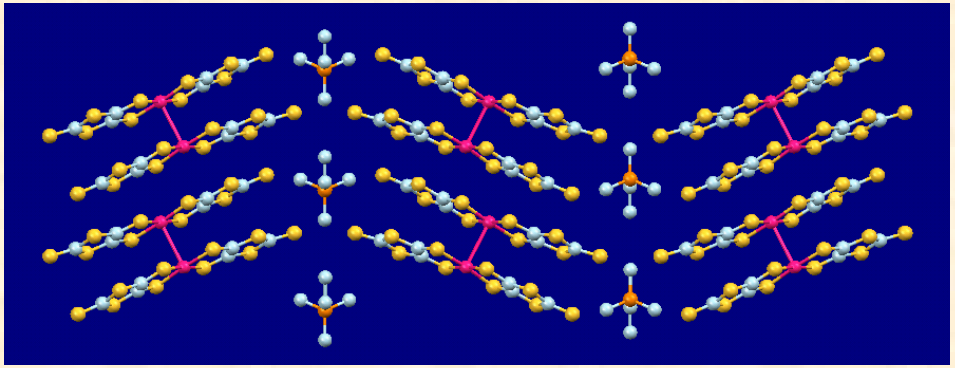




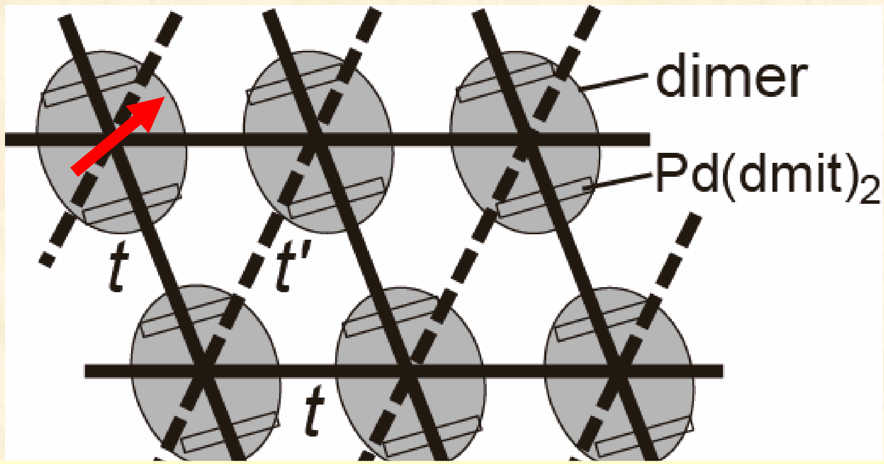
J.A.Schlueter et al, 2004

X[Pd(dmit)$_2$]$_2$



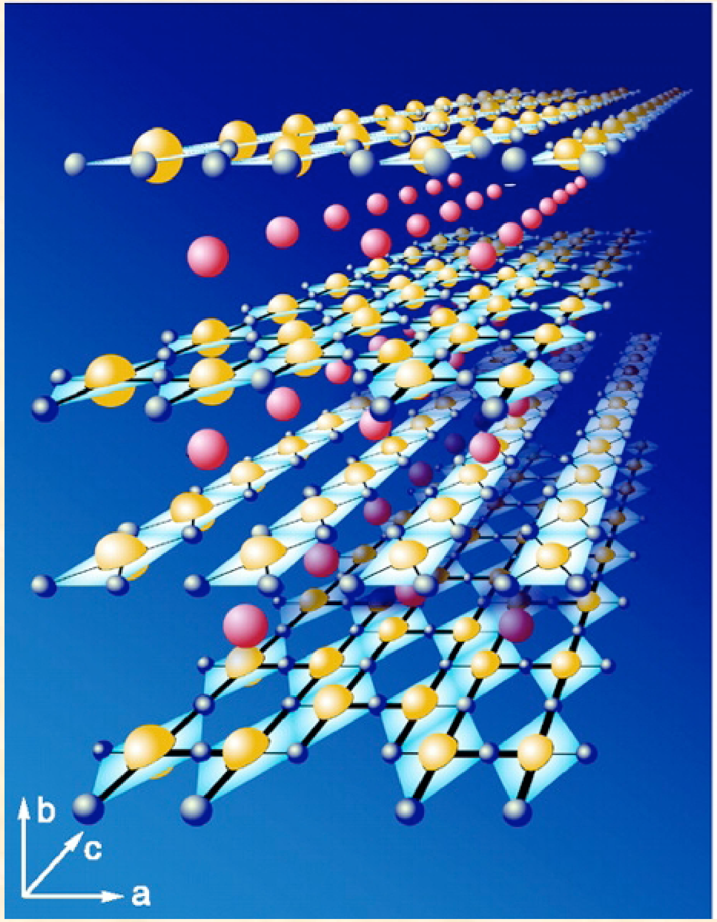


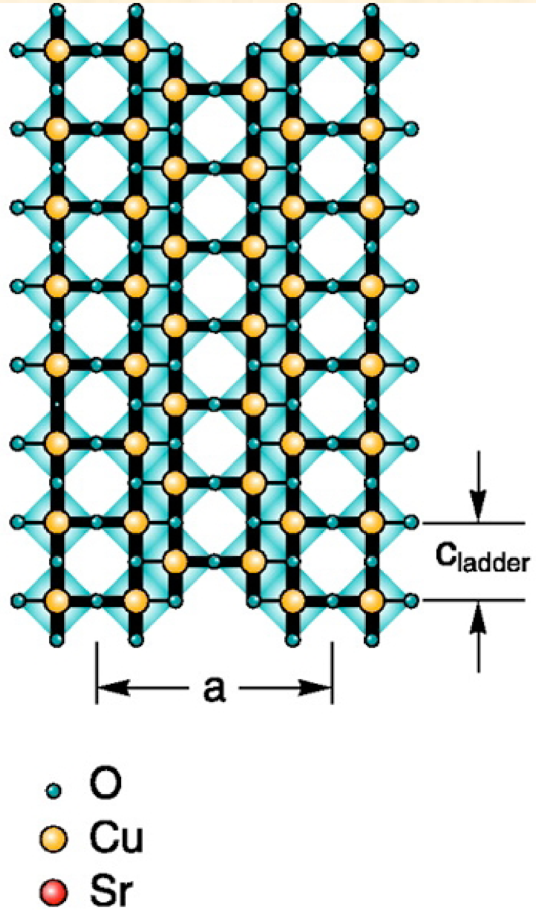
One free electron spin on each vertex of a triangular lattice

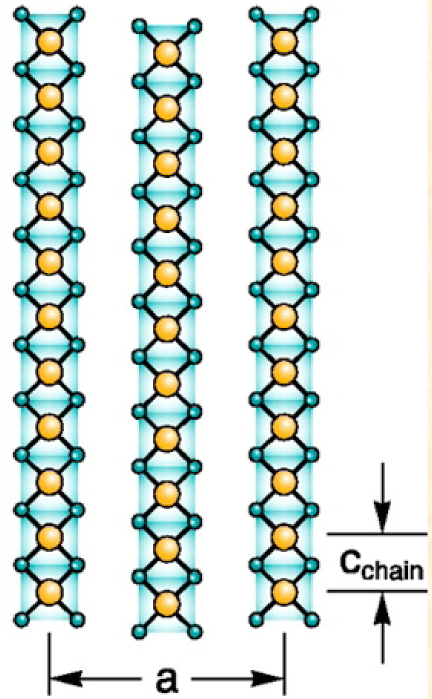


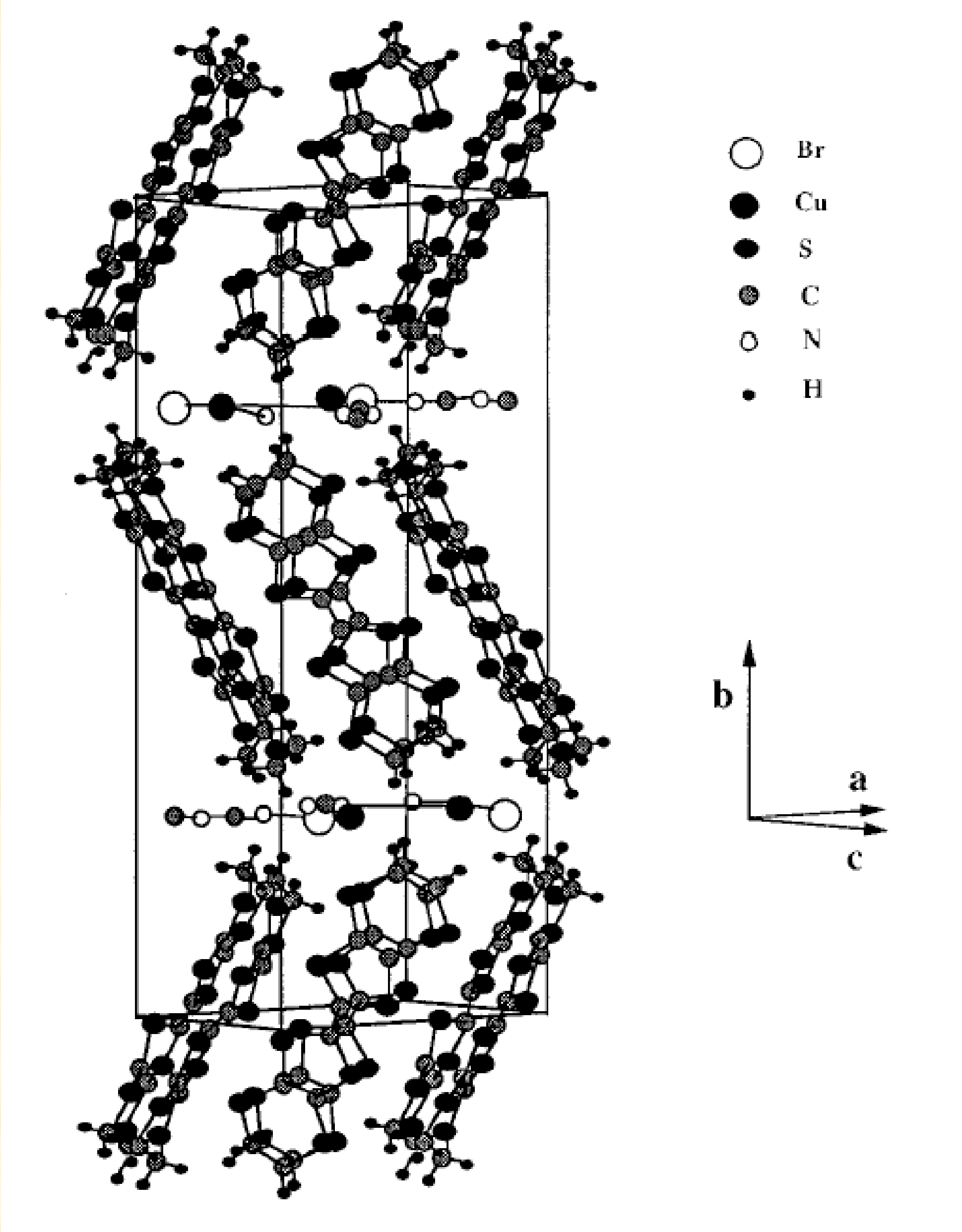
M. Tamura *et al.*, *J. Phys. Soc. Jpn.* **75**, 093701 (2006)

Spin Ladders

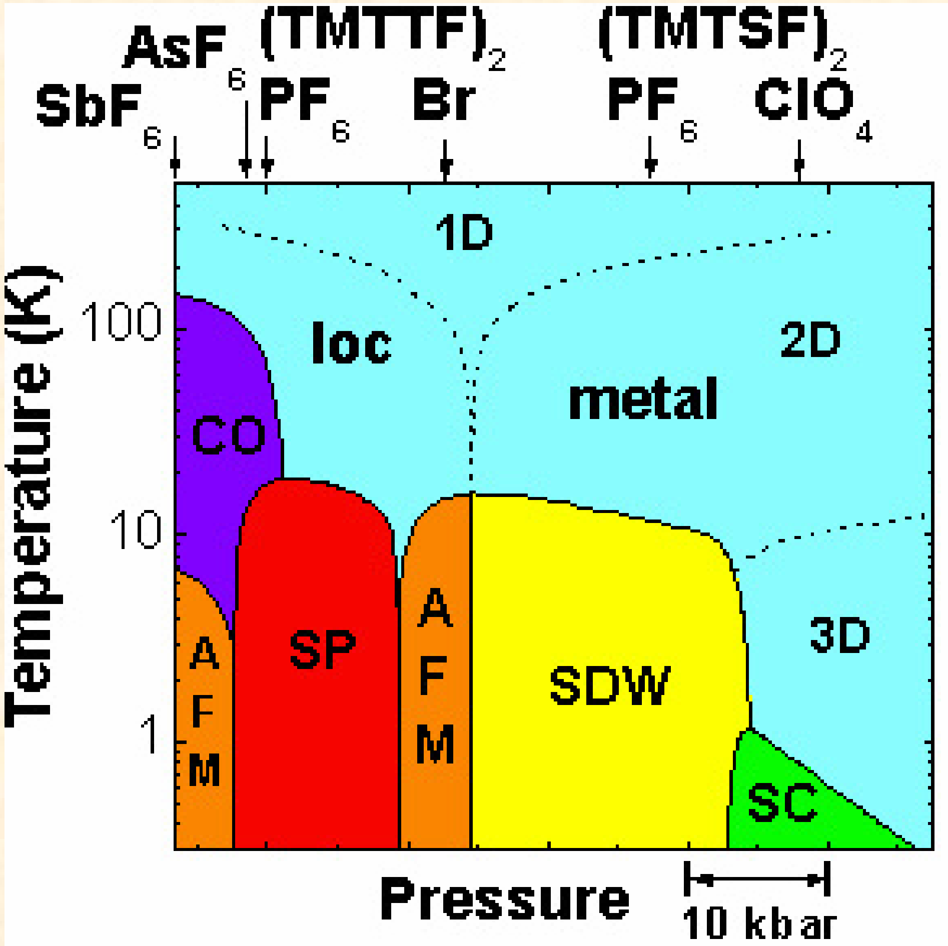







Br
Cu
S
C
N
H
b
a
c

Phase Diagram



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