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ICTP 40th Anniversary

SMR.1572 - 8

Workshop on
Novel States and Phase Transitions in Highly Correlated Matter

12 - 23 July 2004

MnSi, FeSi and CoSi: The strange world of itinerant electrons and local Hunds rule correlations

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MnSi, FeSi and CoSi:
The strange world of itinerant electrons and local Hunds rule correlations

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A. Poteryaev, Universiteit Nijmegen
J.A. Mydosh, MPI Dresden
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J.F. DiTusa, Lousiana State University, Baton Rouge
F. Parmigiani, M . Zangrando , Elettra, Trieste

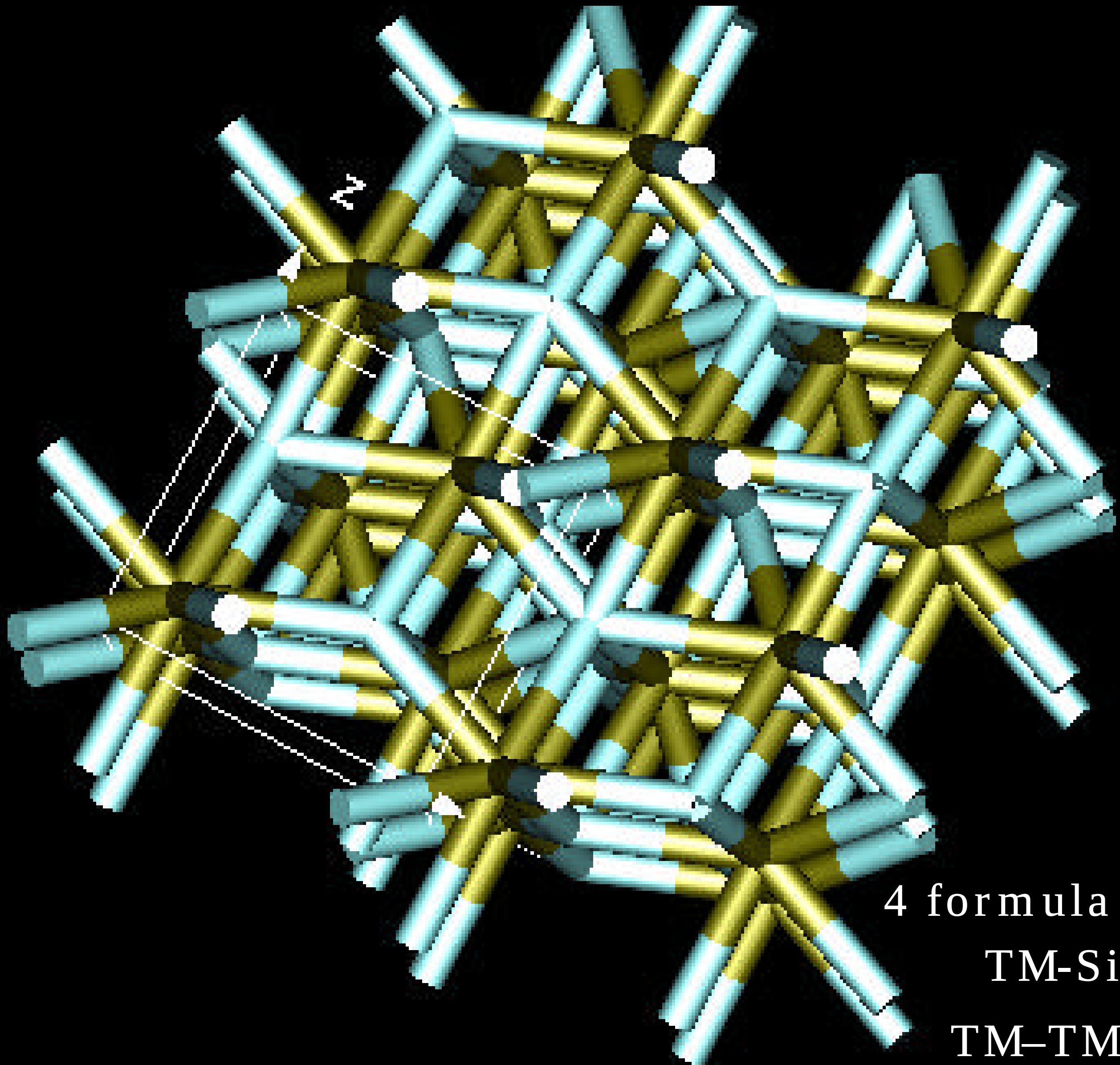
Outline:

$Fe_{1-x}Co_xSi$

MnSi

Conclusions

CrSi, MnSi, FeSi, CoSi, RuSi, RhSi, ReSi, OsSi, FeGe & alloys



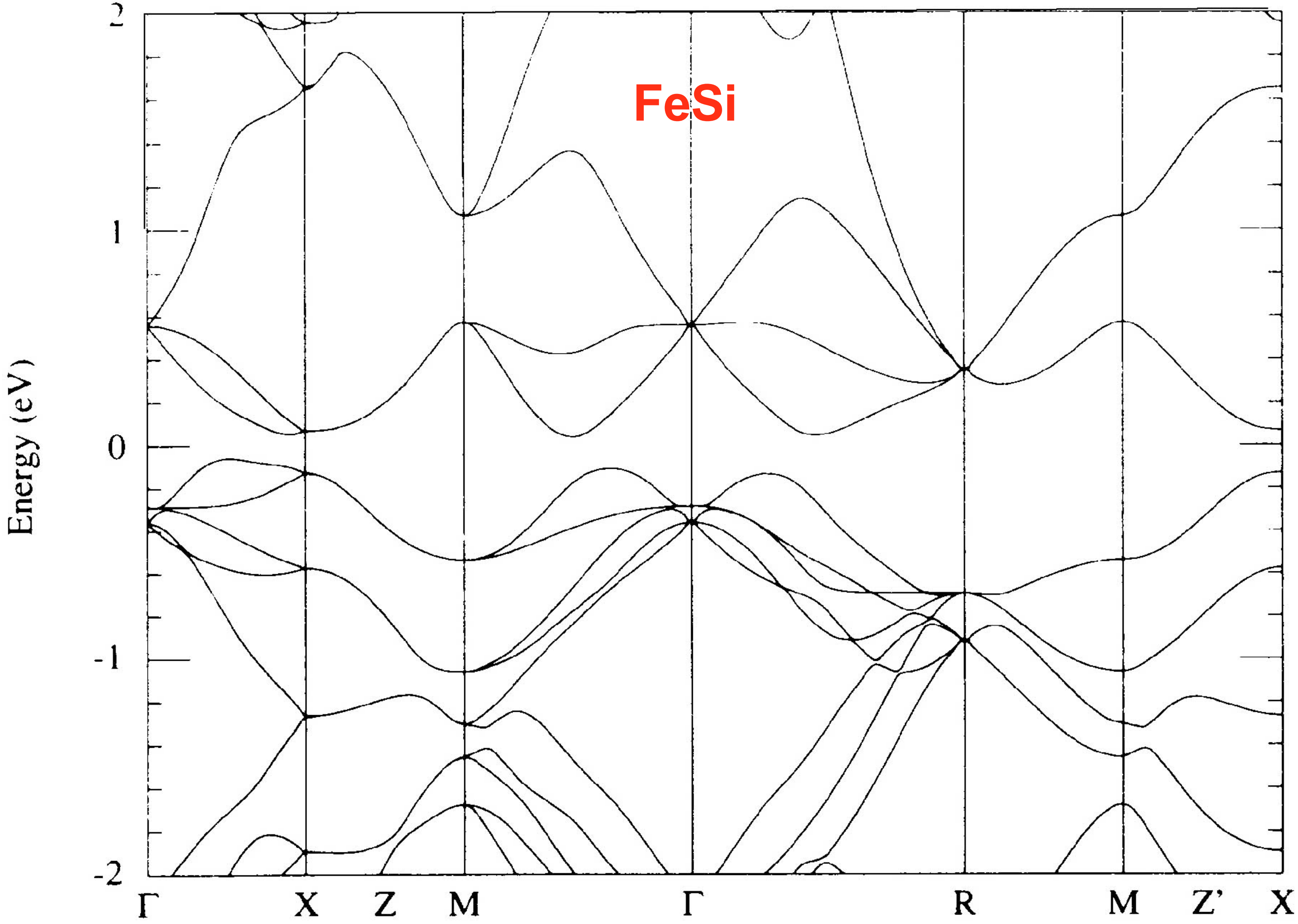
Simple Cubic

T^4-$P2_13$

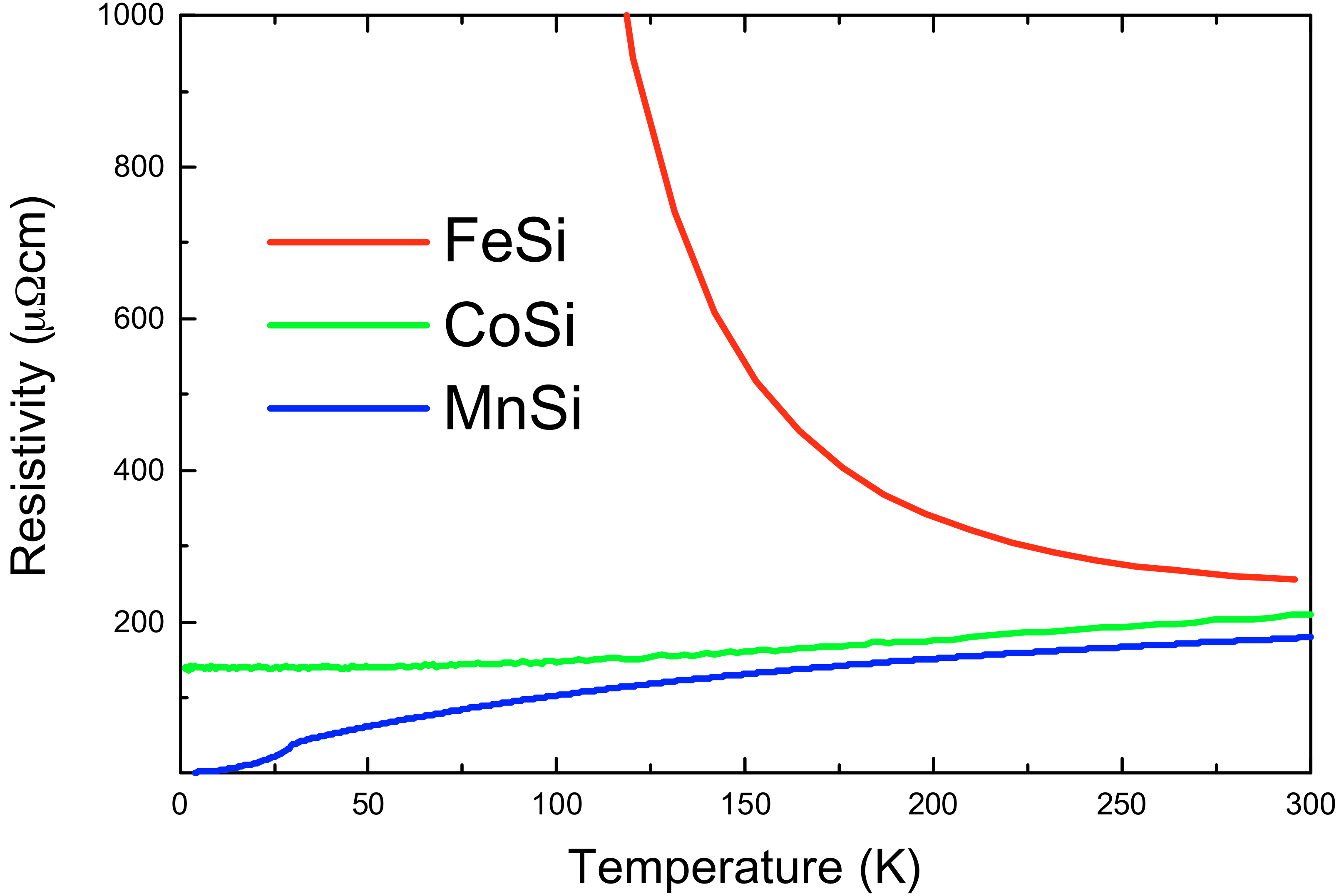
4 formula units / unit cell

TM-Si Coordination=7

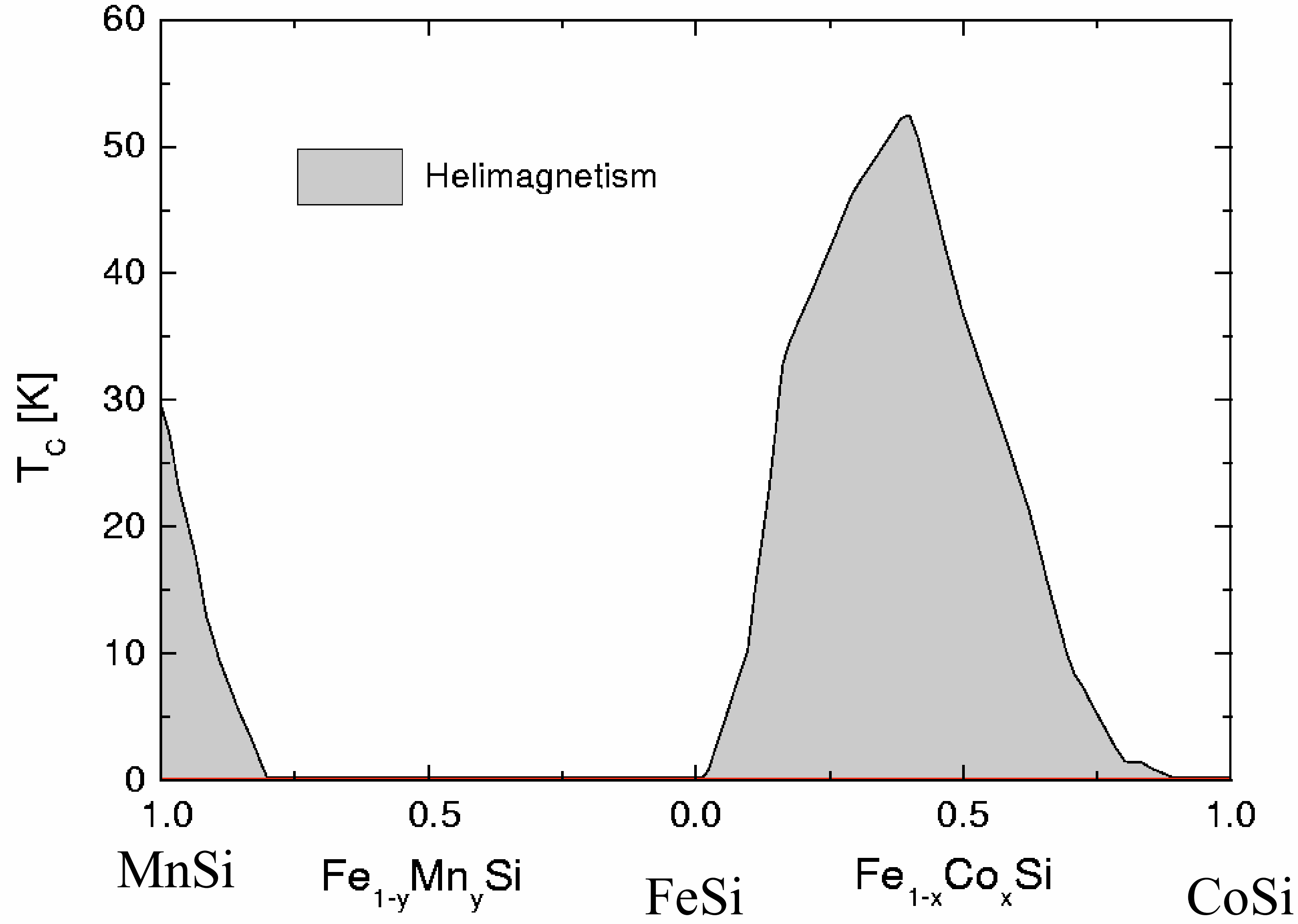
TM–TM Coordination=6



Mattheiss, Hamann, PRB 47 (1993)
Fu, Krijn, Doniach, PRB 49 (1994)

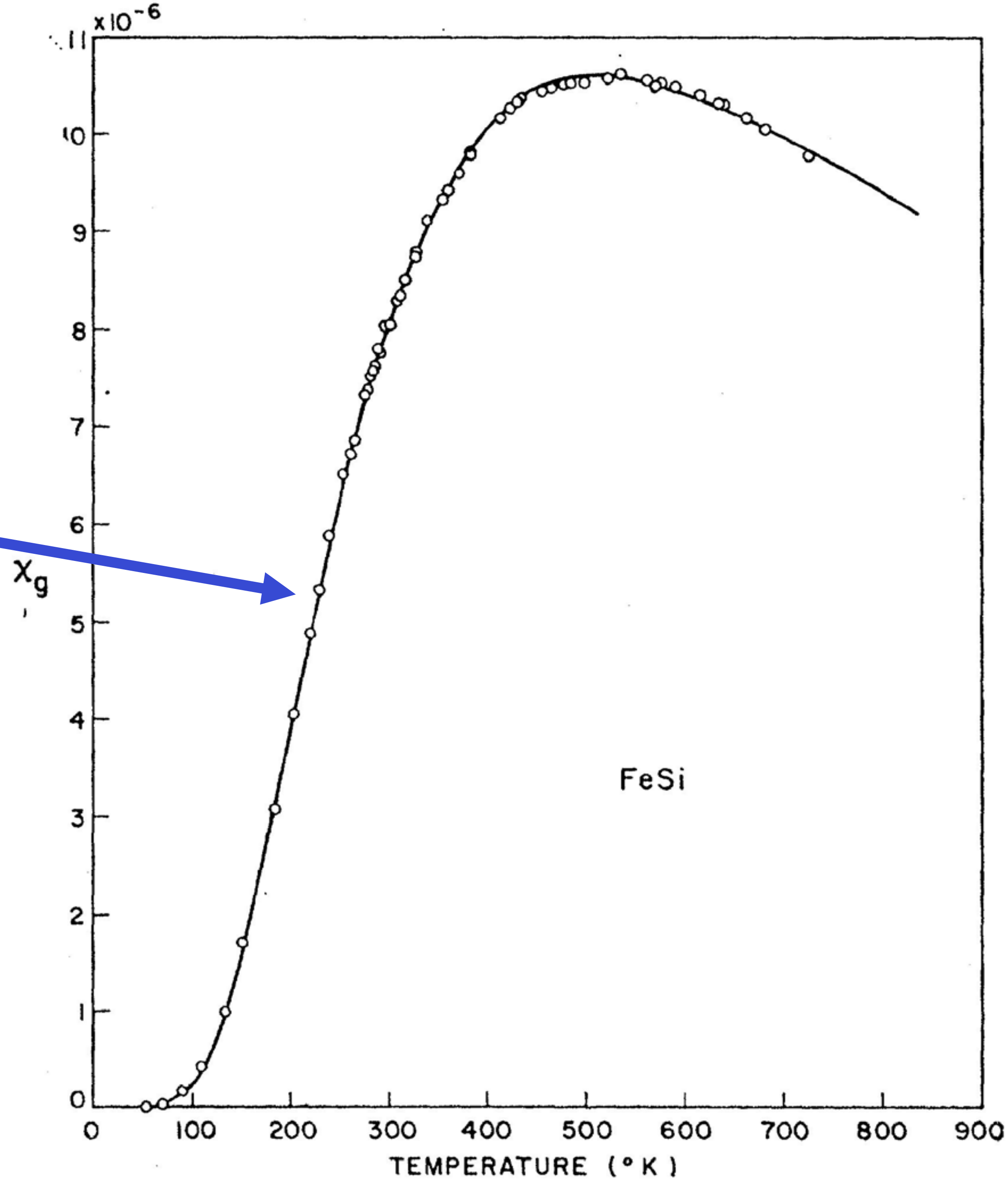


Resistivity (μΩcm)
1000
800
600
400
200
0
50
100
150
200
250
300
Temperature (K)
FeSi
CoSi
MnSi

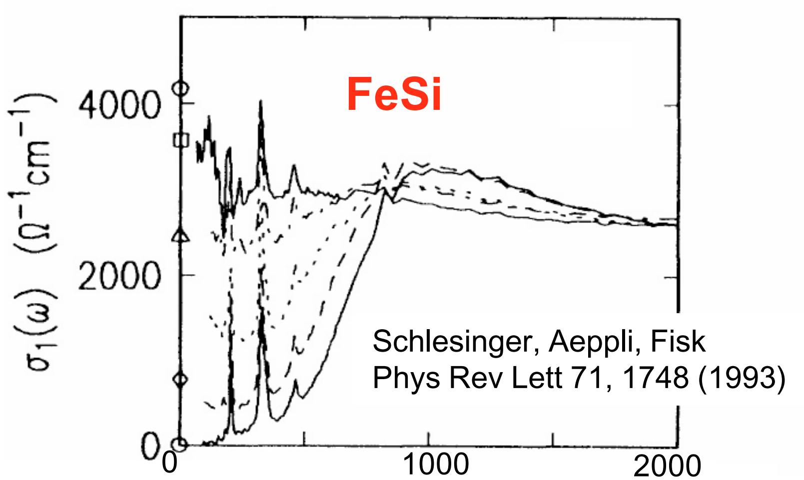


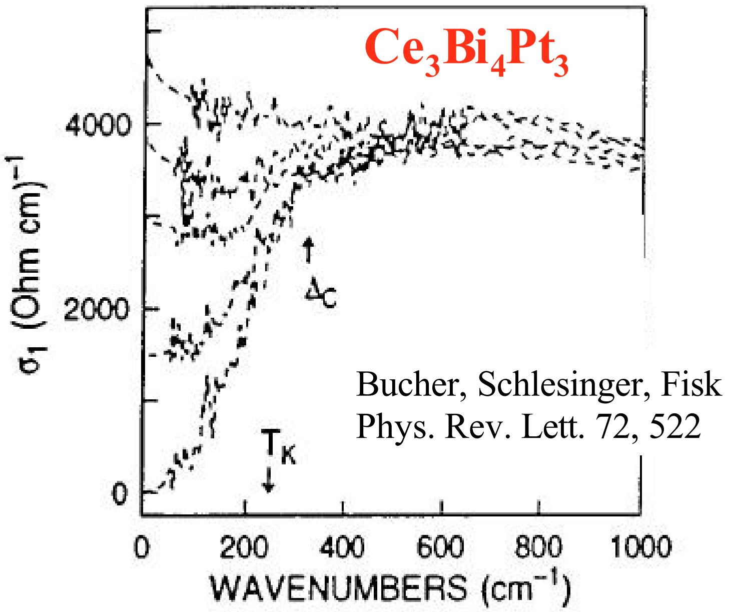
N. Manyala, Y. Sidis, J. F. DiTusa, G. Aeppli, D. P. Young and Z. Fisk,
Nature 404, 581 (2000).

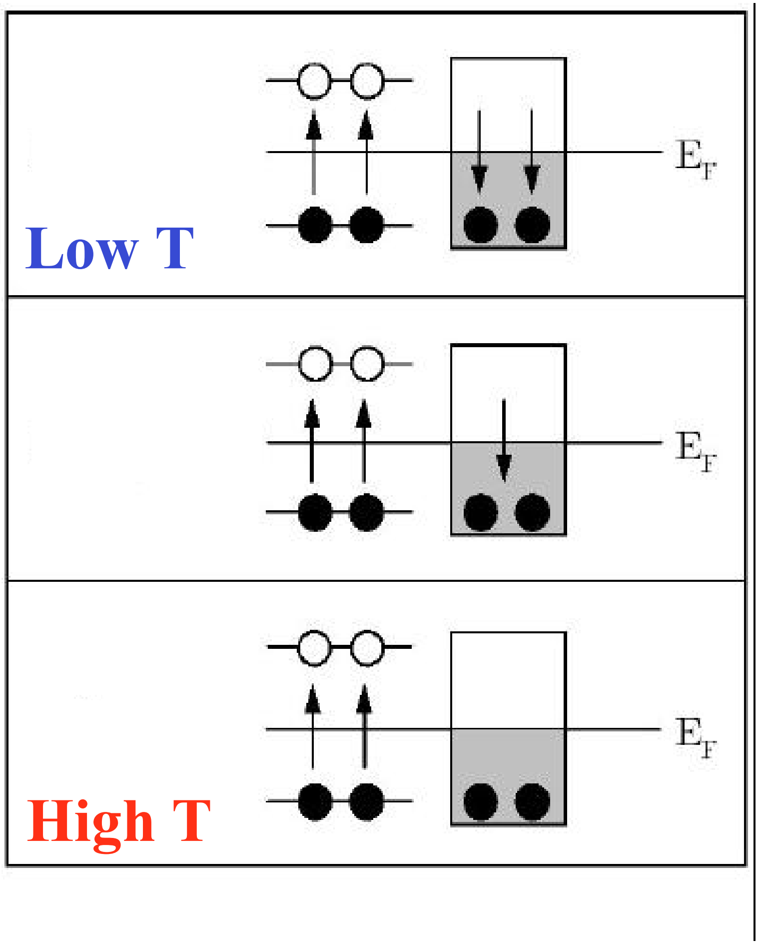
V.Jaccarino, et al,
Phys Rev 160 (1967)
Δ_s=750 K



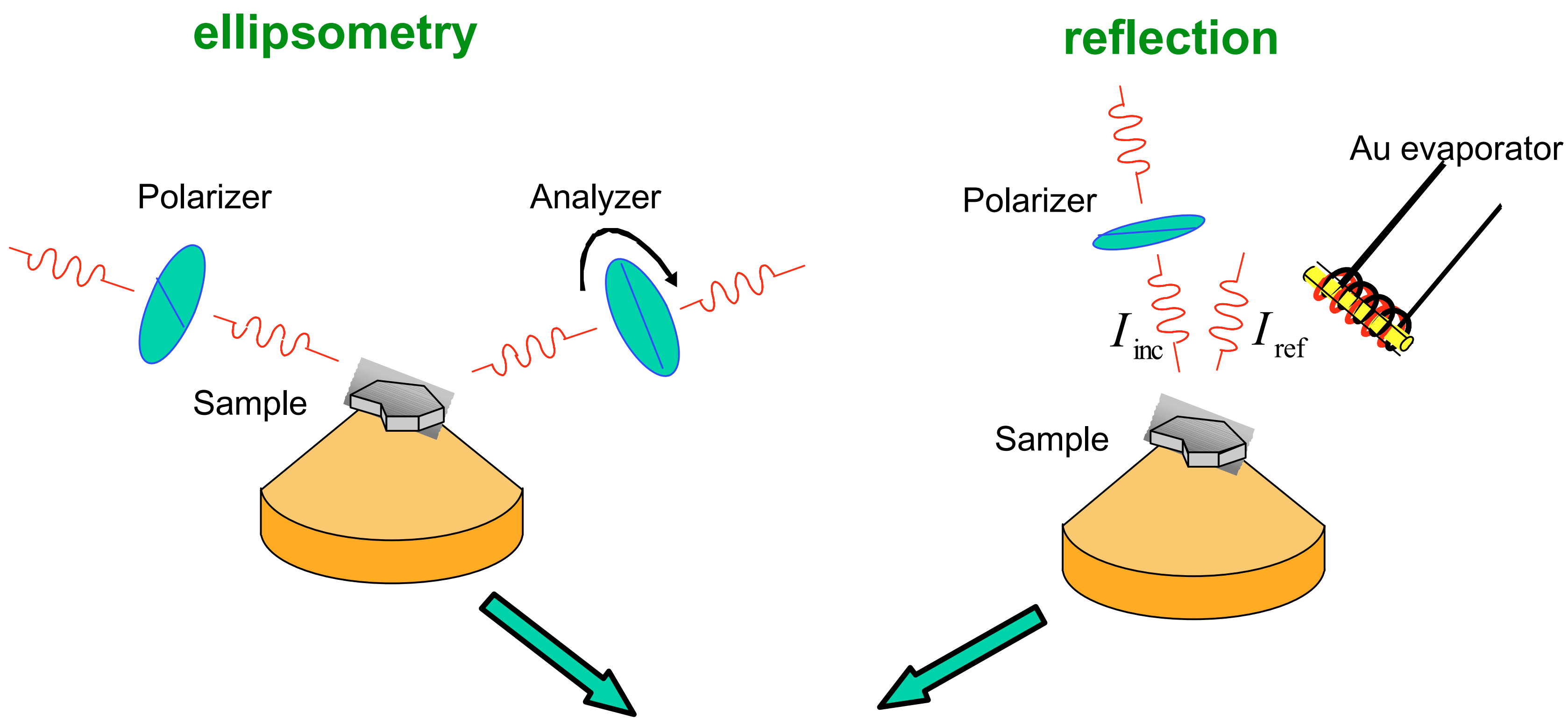
FeSi: a Kondo Lattice ?





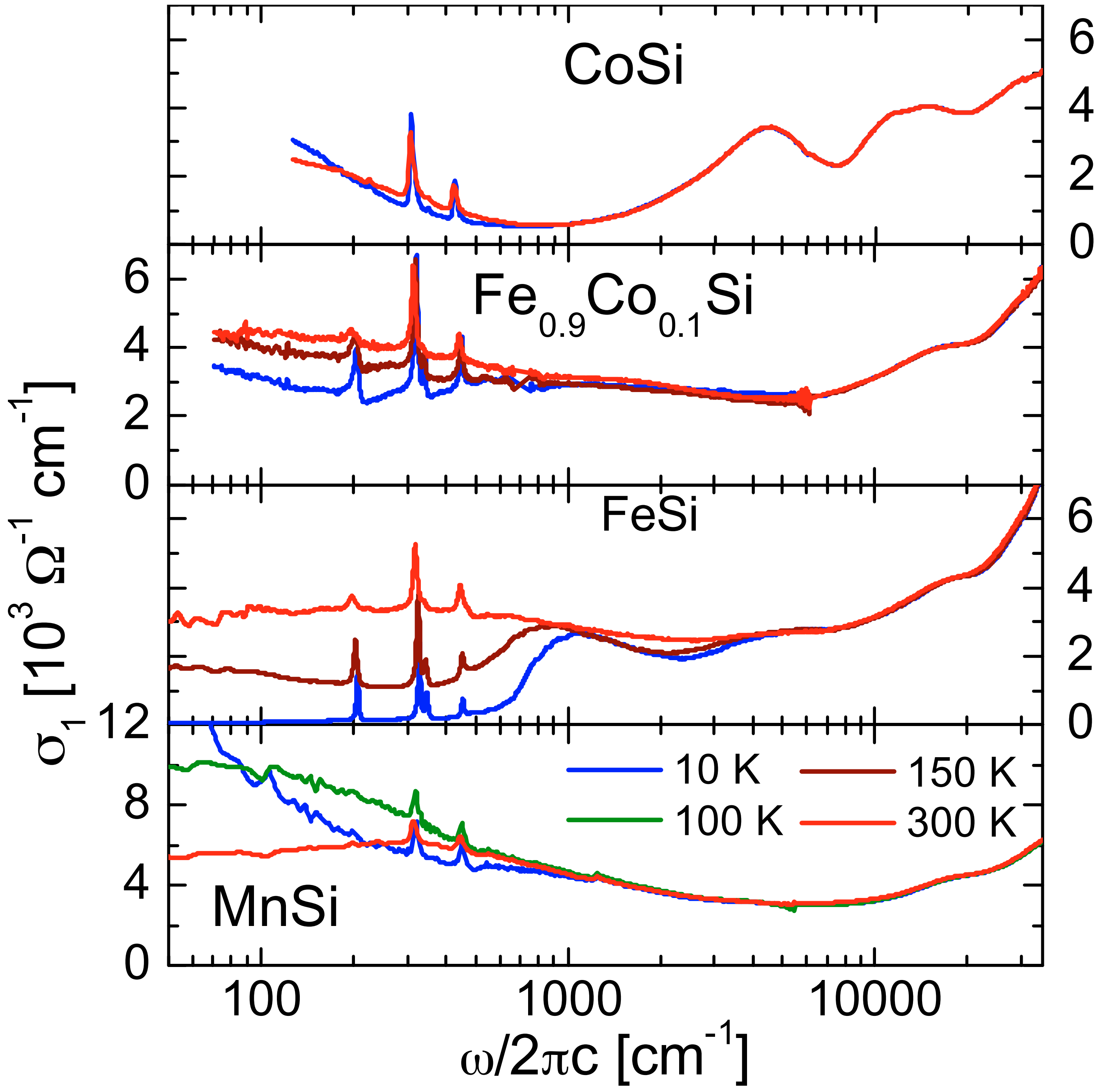


Optical techniques

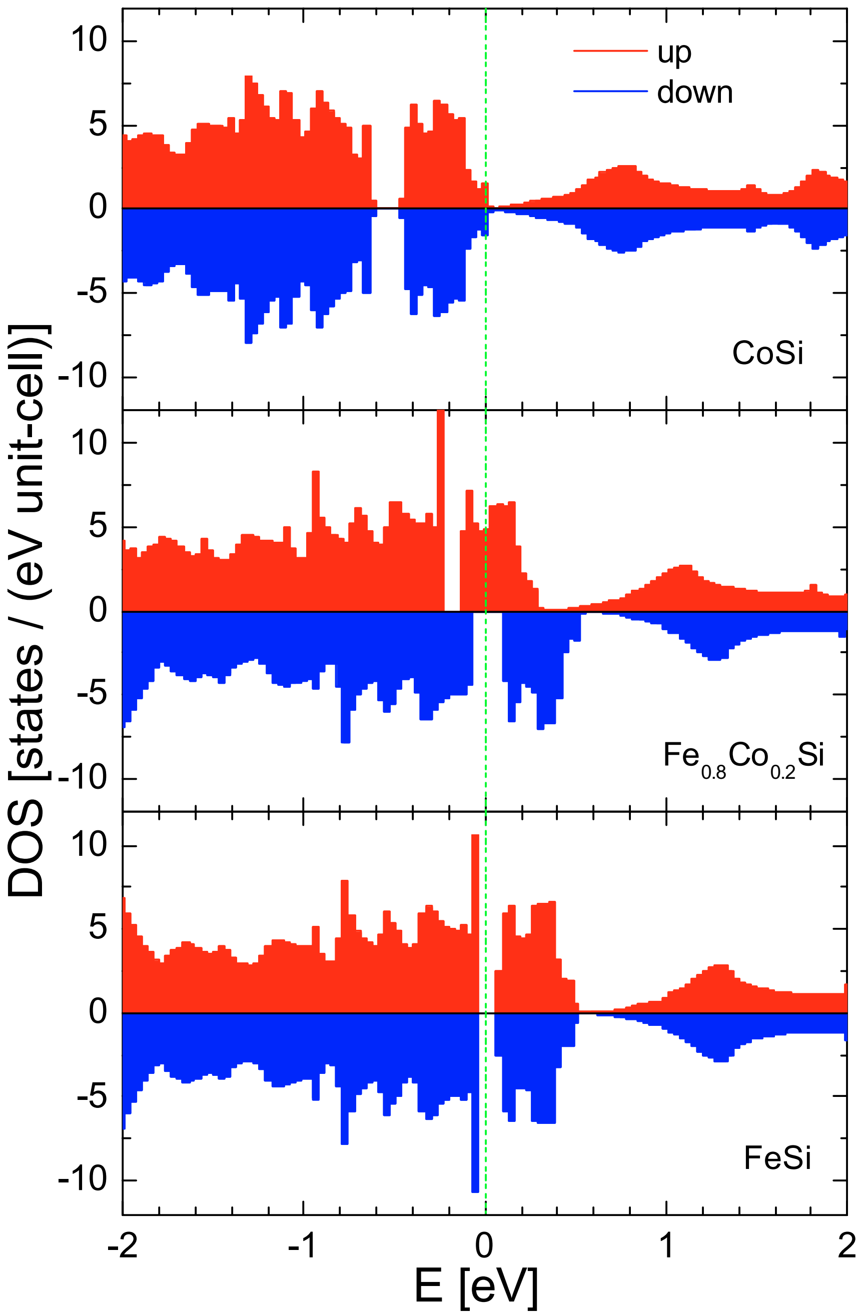


Optical conductivity

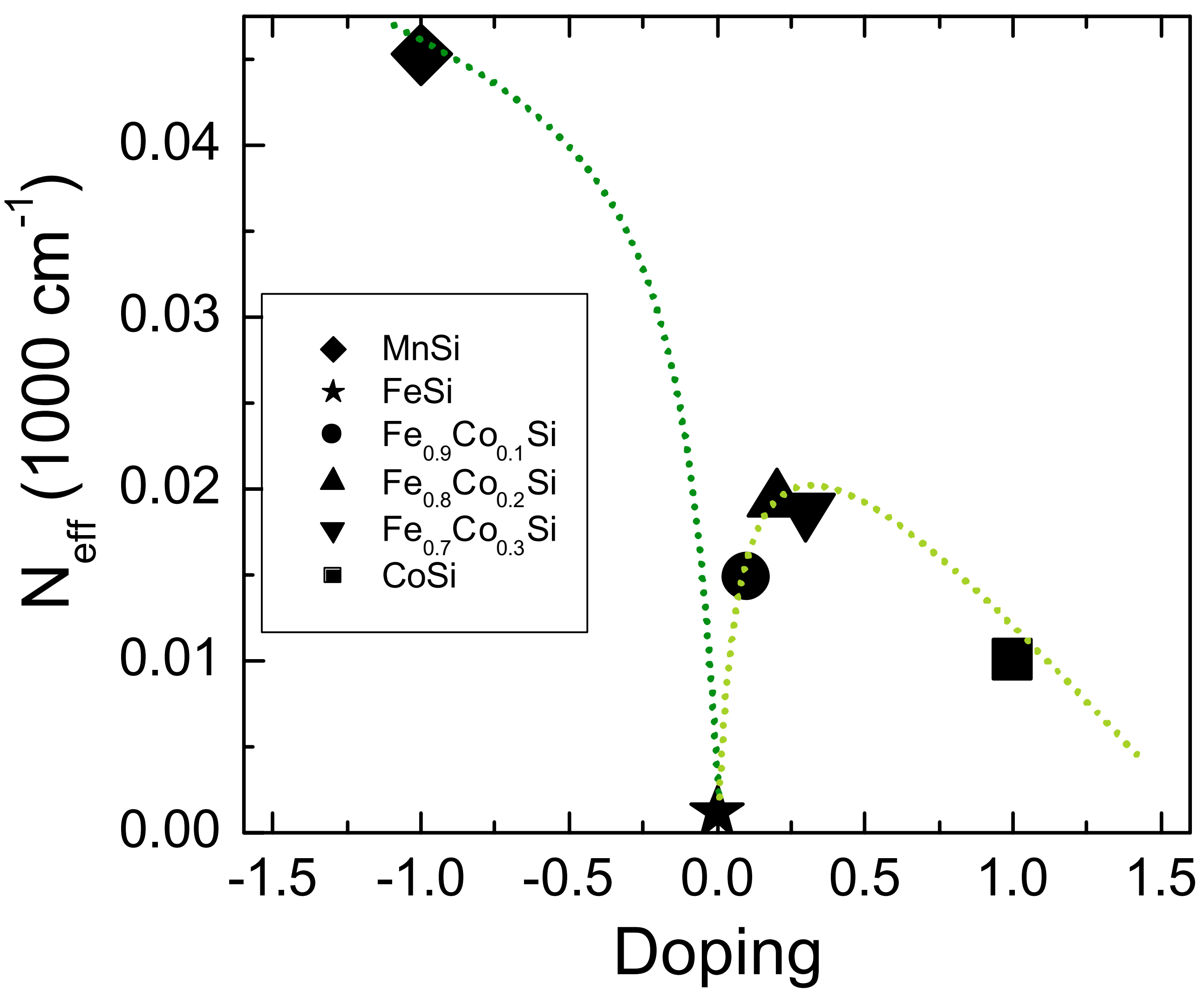
$\sigma_1(\omega) + i\,\sigma_2(\omega)$



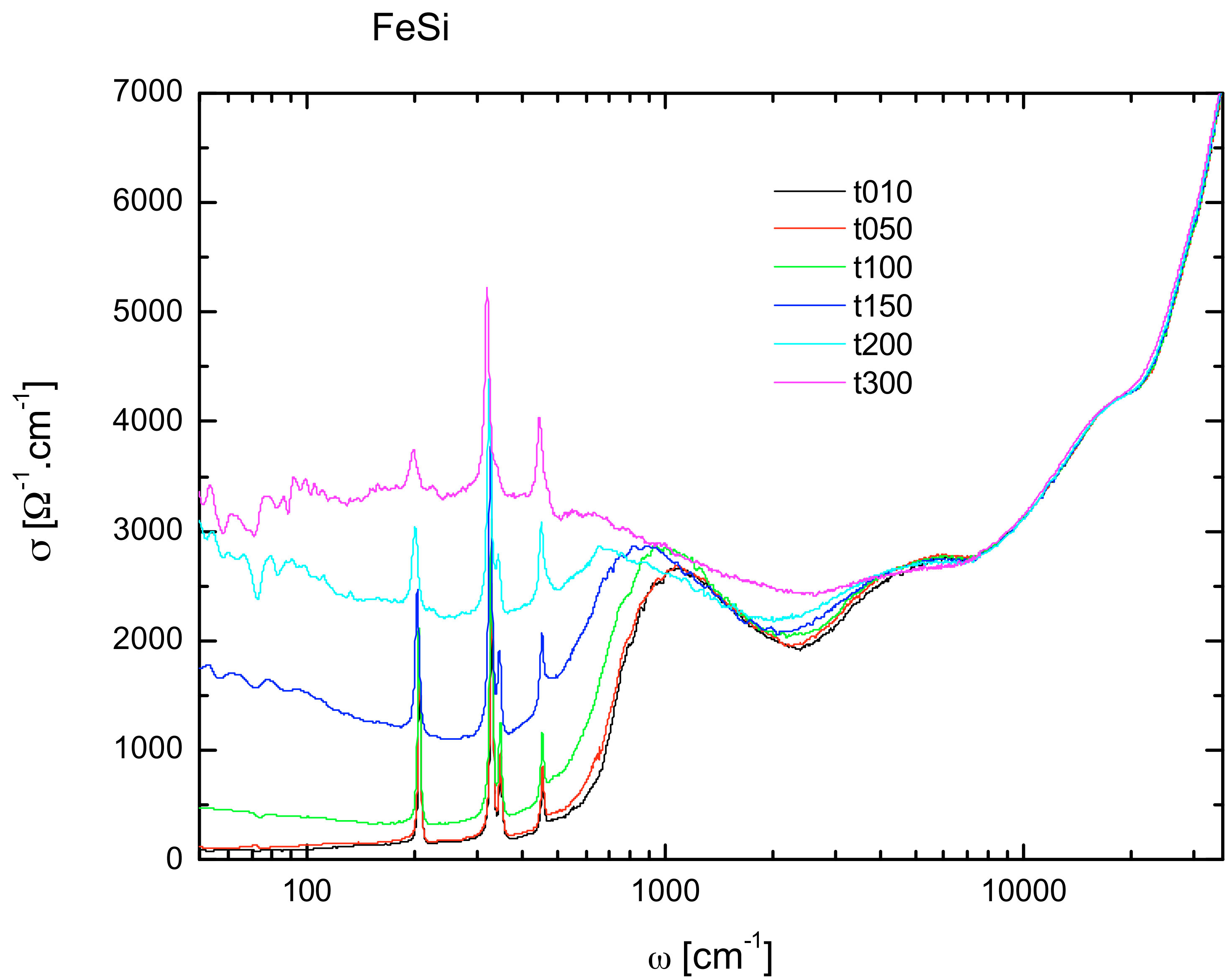
CoSi
Fe0.9Co0.1Si
FeSi
MnSi
10 K
100 K
150 K
300 K
σ1 [10^3 Ω^-1 cm^-1]
ω/2πc [cm^-1]
100
1000
10000
0
2
4
6
8
12



up
down
CoSi
$Fe_{0.8}Co_{0.2}Si$
FeSi
DOS [states / (eV unit-cell)]
E [eV]

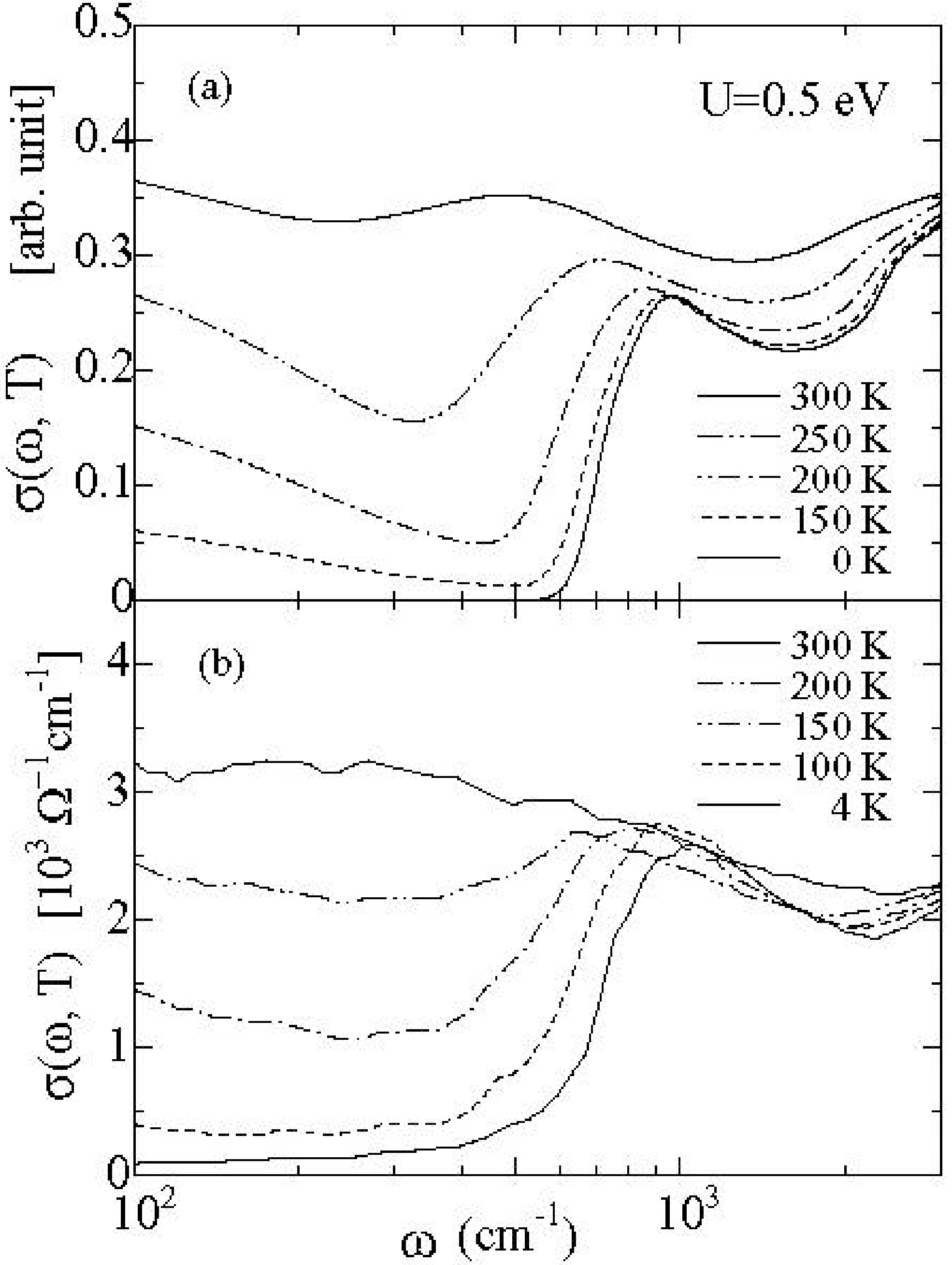


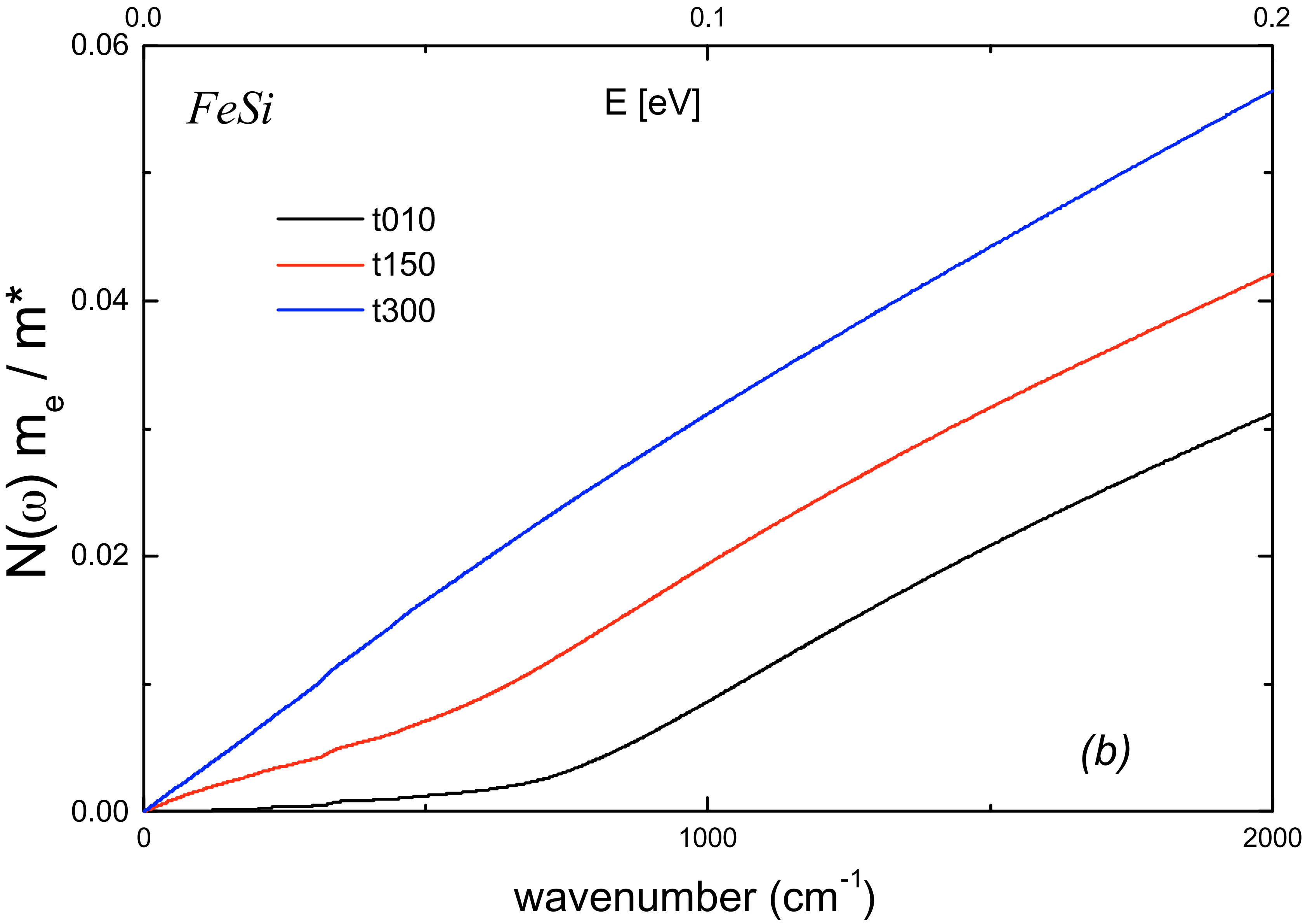
MnSi
FeSi
$Fe_{0.9}Co_{0.1}Si$
$Fe_{0.8}Co_{0.2}Si$
$Fe_{0.7}Co_{0.3}Si$
CoSi
N_{eff} (1000 cm^{-1})
0.00
0.01
0.02
0.03
0.04
-1.5
-1.0
-0.5
0.0
0.5
1.0
1.5
Doping


FeSi
t010
t050
t100
t150
t200
t300
σ [Ω-1.cm-1]
ω [cm-1]
0
1000
2000
3000
4000
5000
6000
7000
100
1000
10000

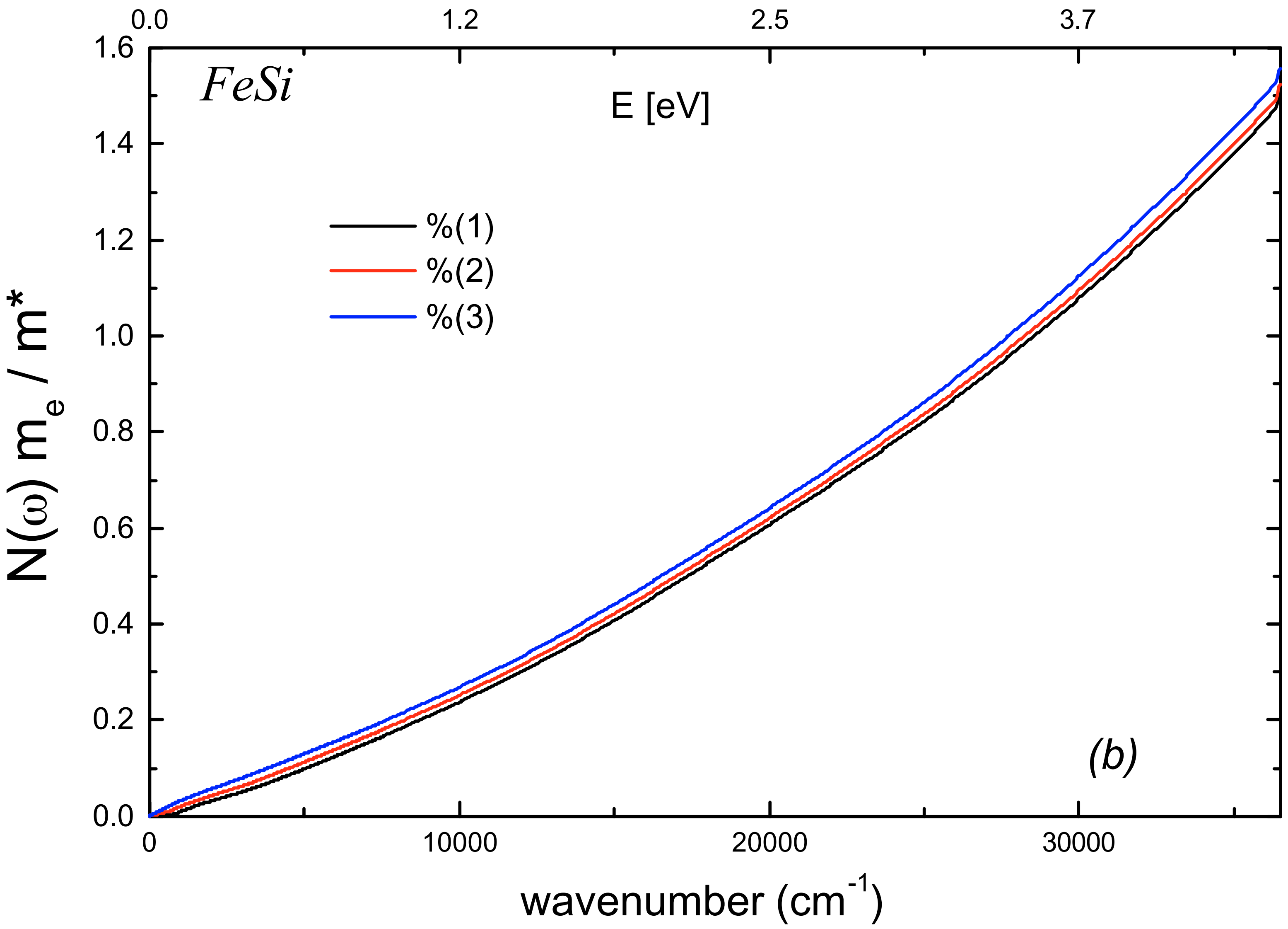
K. Urasaki & T. Saso,
Physica B 281 (1999)

2-band Hubbard
U=0.5 eV
DMFT
+
self consistent
renormalization

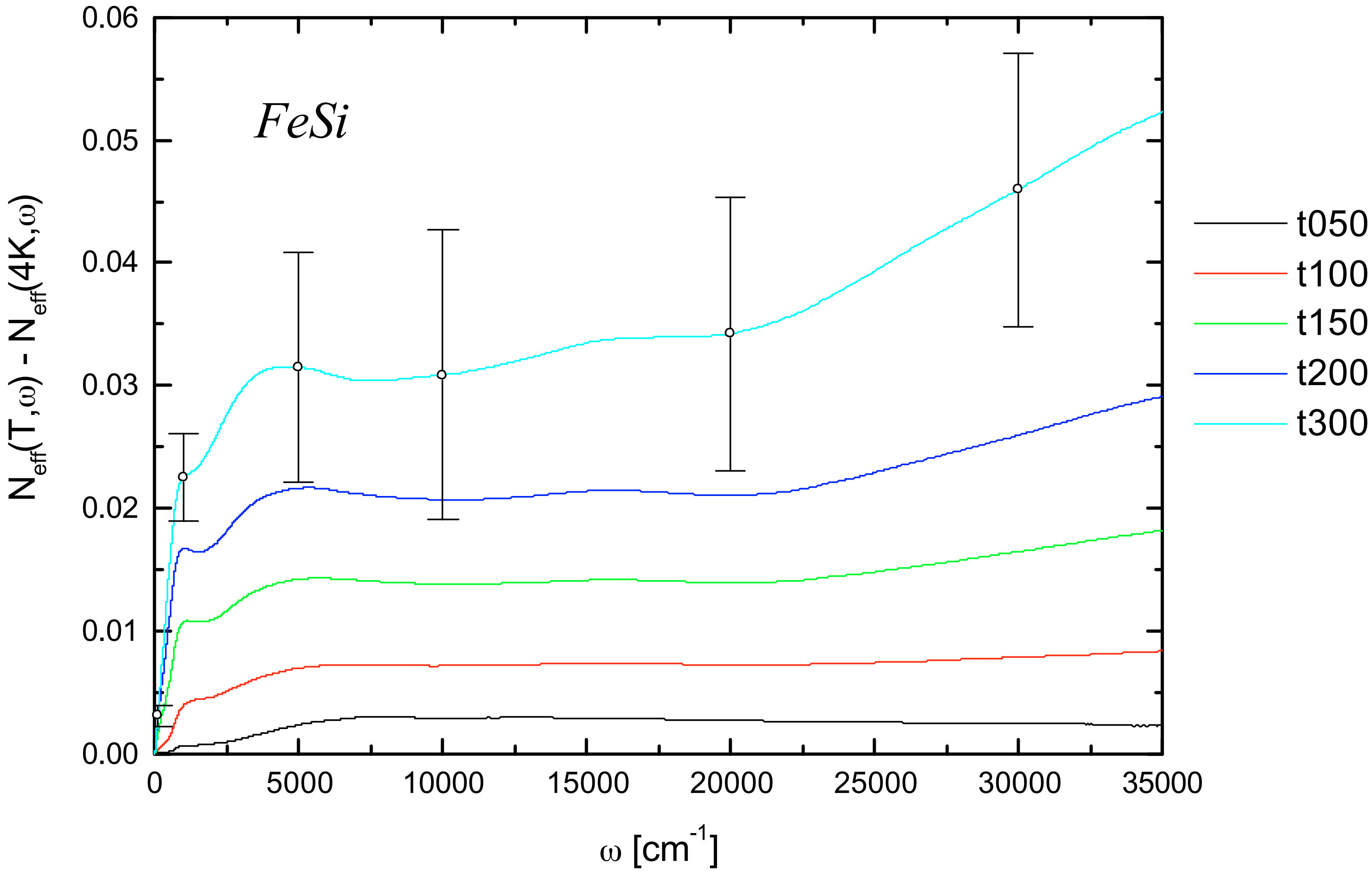




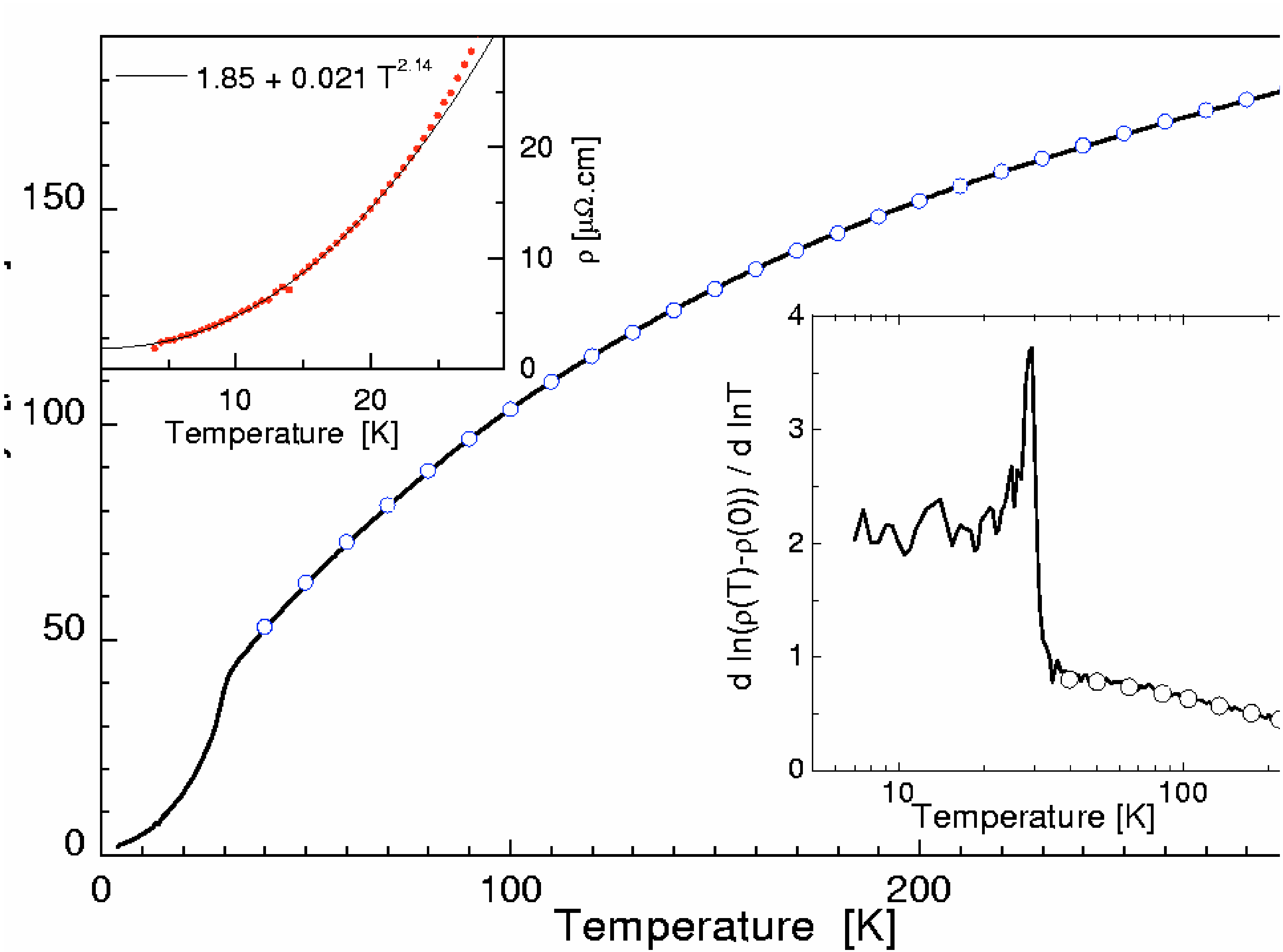
0.0
0.1
0.2
E [eV]
FeSi
t010
t150
t300
(b)
0.06
0.04
0.02
0.00
N(ω) m_e / m*
0
1000
2000
wavenumber (cm^-1)

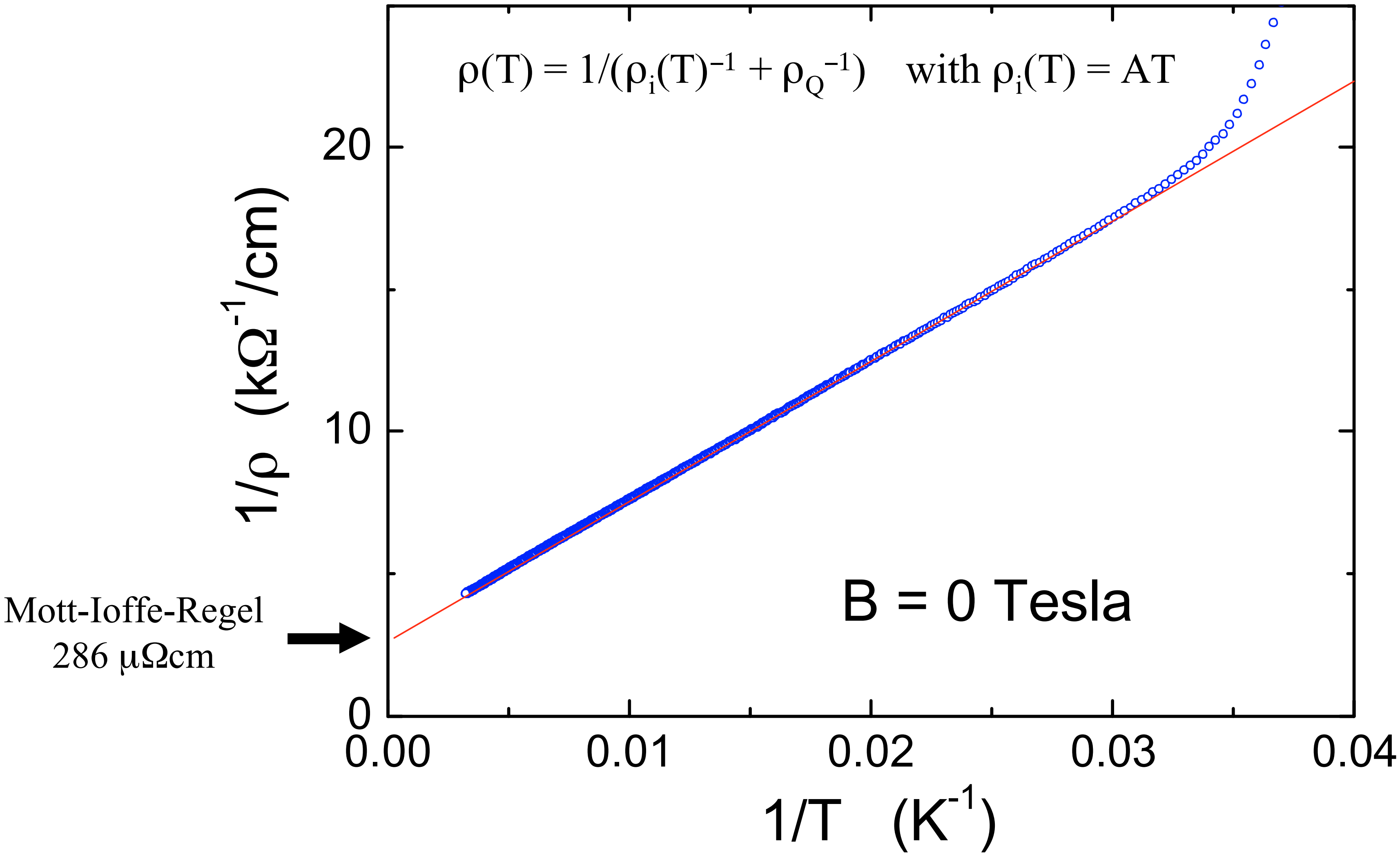


FeSi
E [eV]
0.0
1.2
2.5
3.7
%(1)
%(2)
%(3)
(b)
N(ω) m_e / m*
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
0
10000
20000
30000
wavenumber (cm^-1)

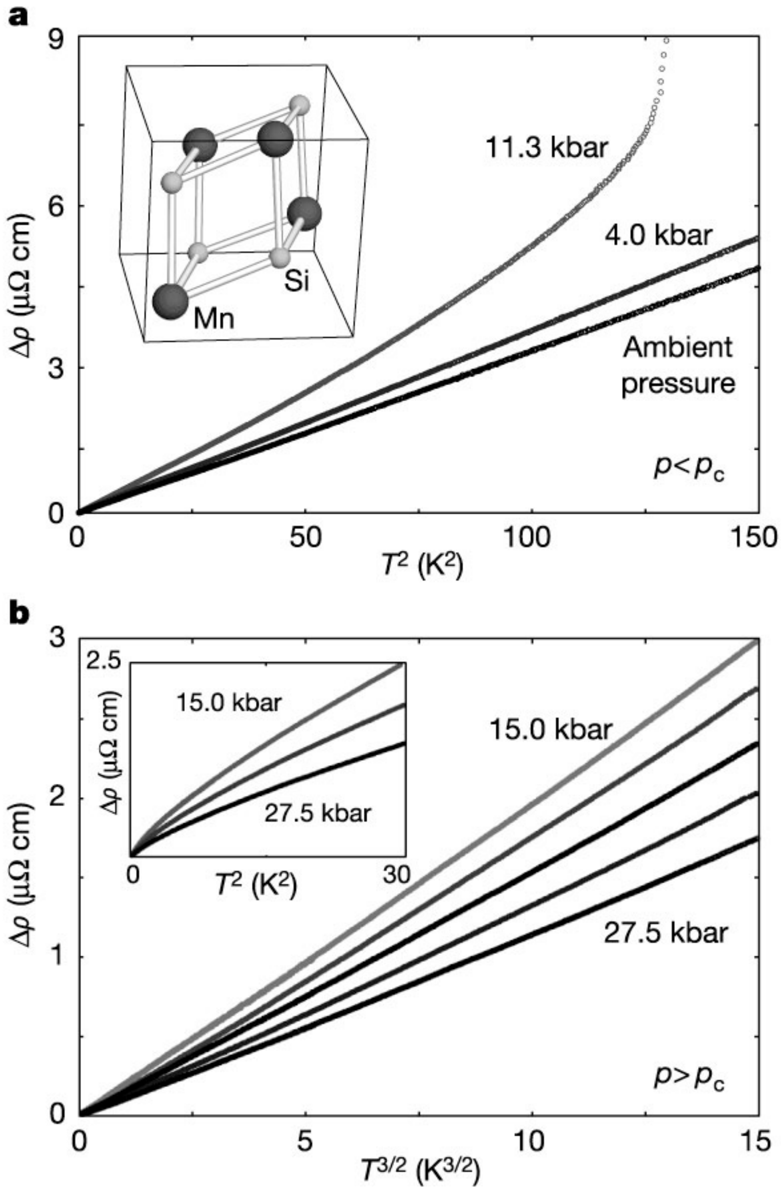


FeSi
0.06
0.05
0.04
0.03
0.02
0.01
0.00
0
5000
10000
15000
20000
25000
30000
35000
N_eff(T,ω) - N_eff(4K,ω)
ω [cm^-1]
t050
t100
t150
t200
t300

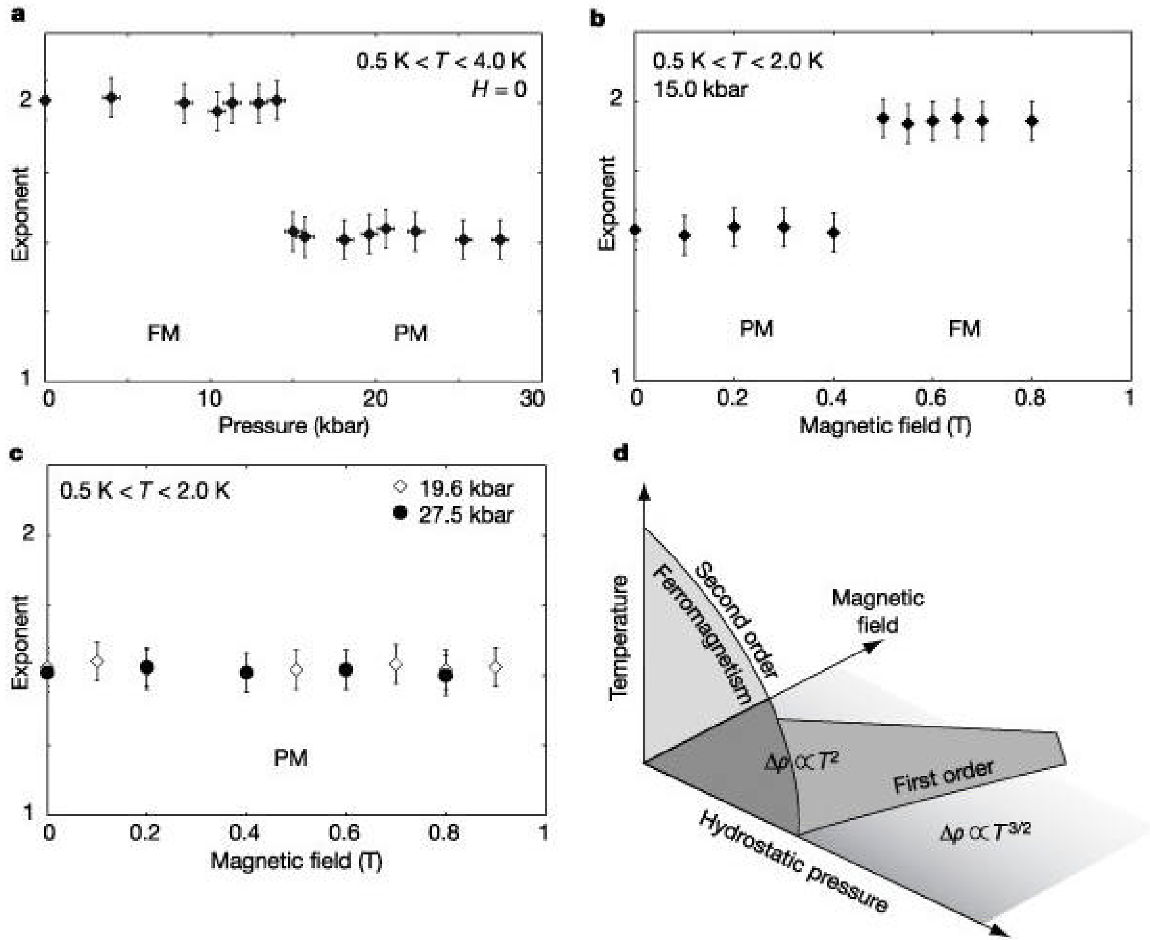

1.85 + 0.021 T^2.14
ρ [μΩ.cm]
Temperature [K]
d ln(ρ(T)-ρ(0)) / d lnT
Temperature [K]
Temperature [K]
0
50
100
150
0
100
200
10
20
0
10
20
0
1
2
3
4
10
100



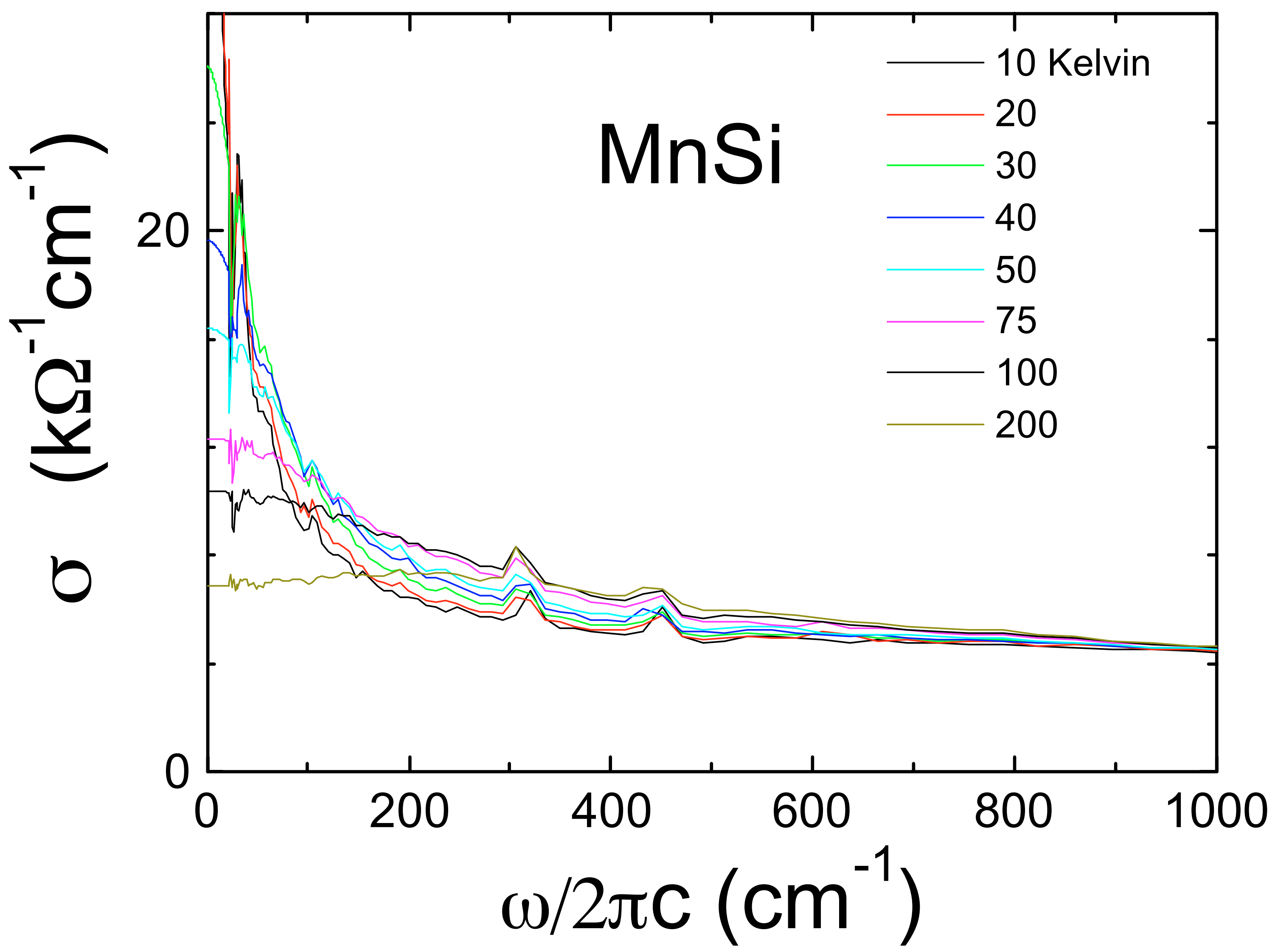
ρ(T) = 1/(ρ_i(T)^{−1} + ρ_Q^{−1}) with ρ_i(T) = AT
B = 0 Tesla
Mott-Ioffe-Regel
286 μΩcm
1/ρ (kΩ^{-1}/cm)
1/T (K^{-1})
0
10
20
0.00
0.01
0.02
0.03
0.04



N. Doiron-Leyraud et al, *Nature* **425**, 595 - 599 (09 Oct 2003)

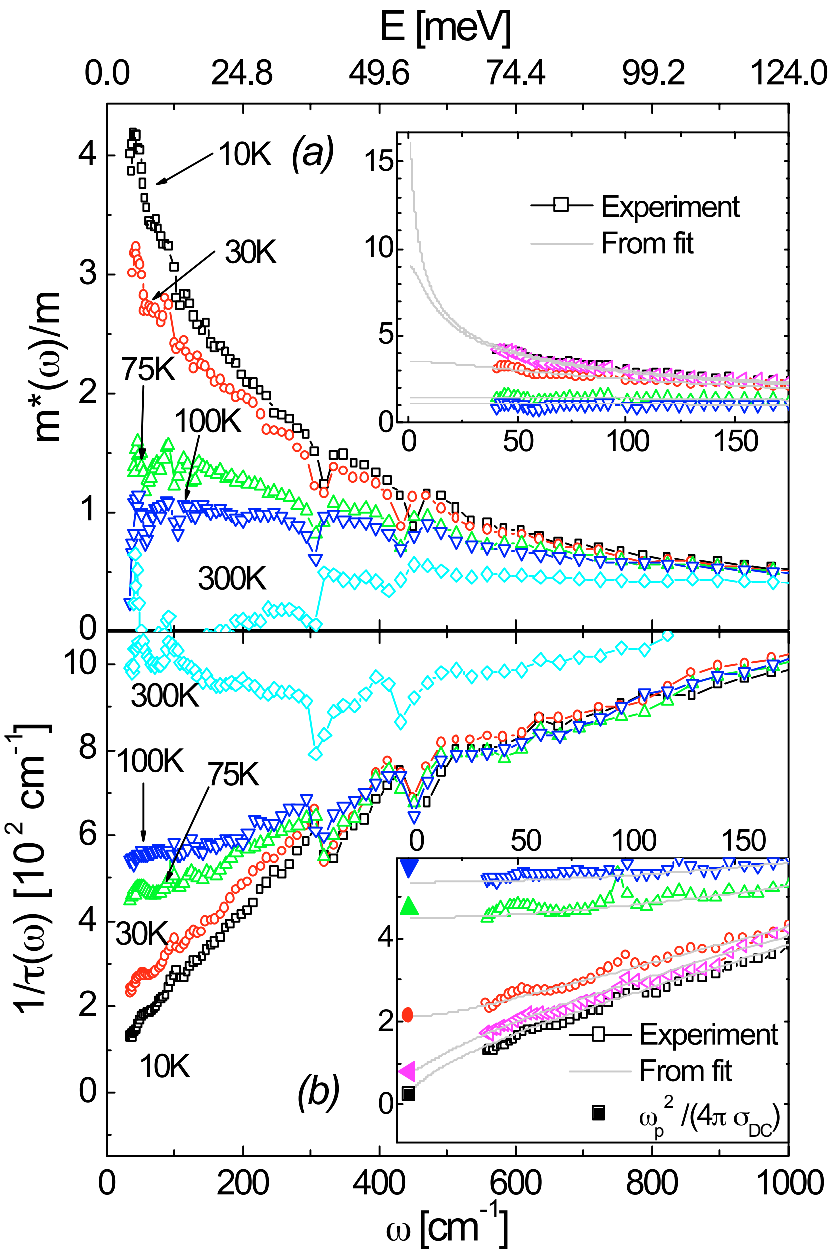


N. Doiron-Leyraud et al, *Nature* **425**, 595 - 599 (09 Oct 2003)



F. P. Mena, D. van der Marel, A. Damascelli, M. Fäth,

A. A. Menovsky, and J. A. Mydosh ,Phys. Rev. B **67**, 241101 (2003)

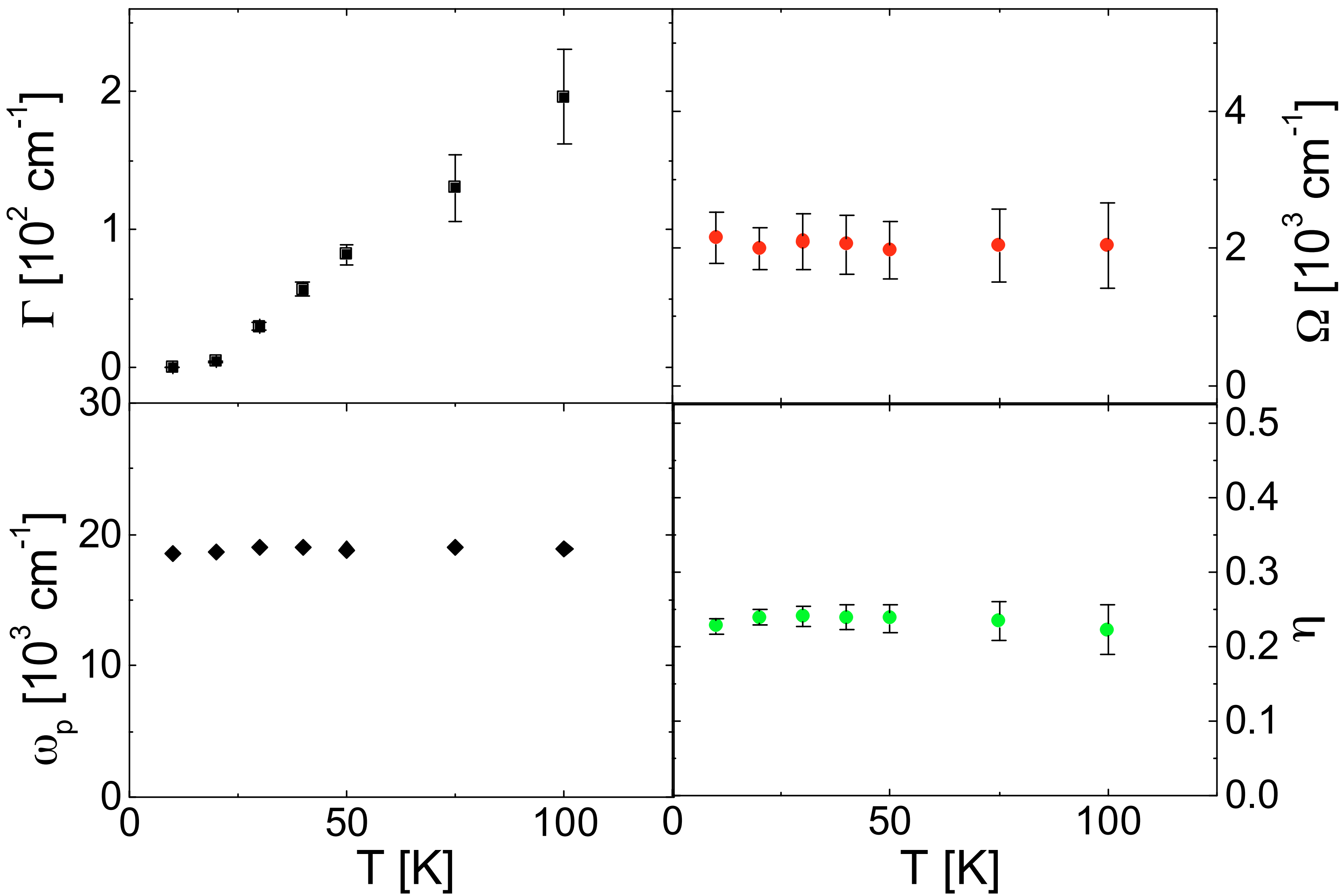


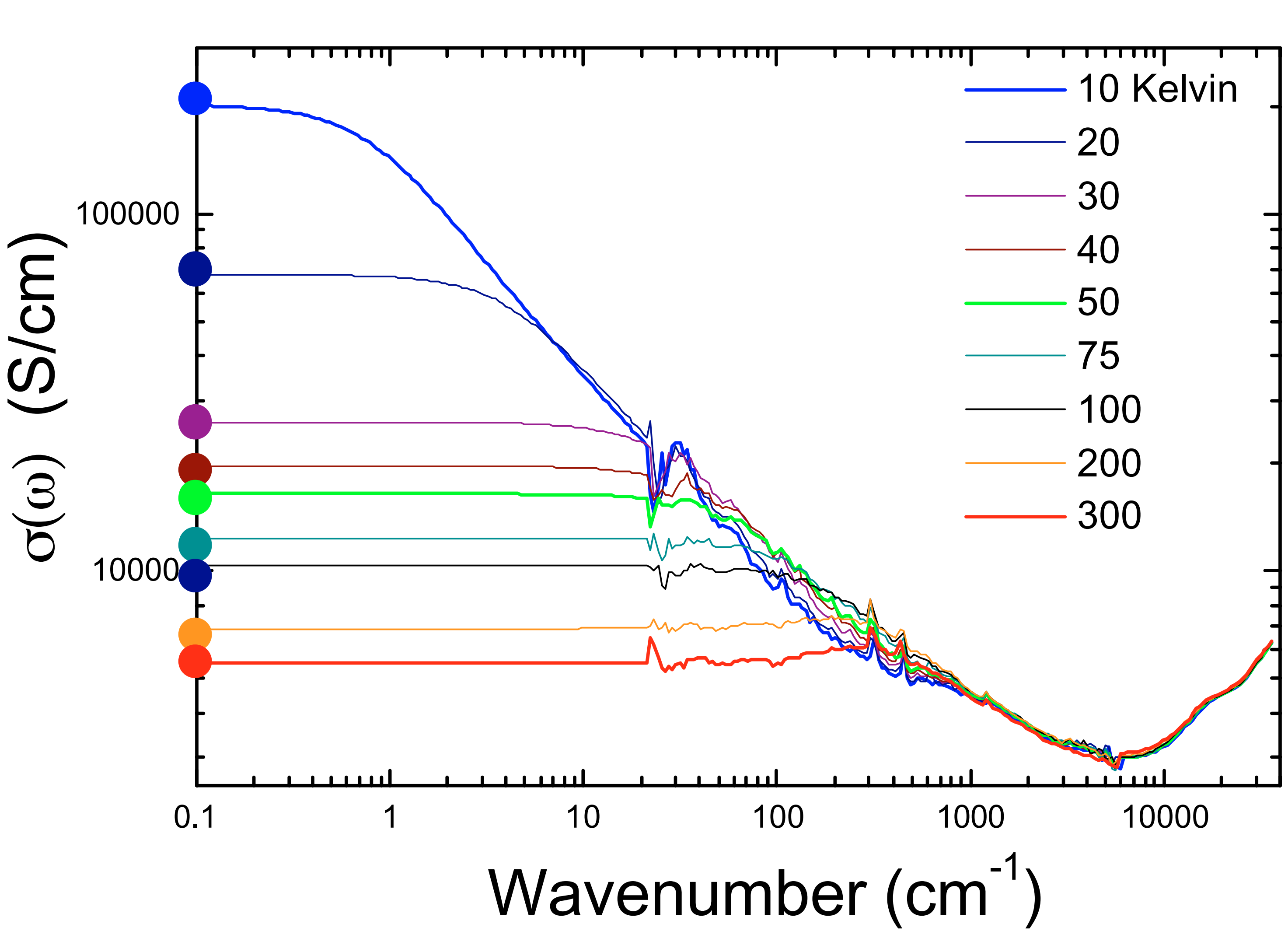
$$\frac{m^*(\omega)}{m} \equiv \mathrm{Im}\frac{-\omega_p^2/4\pi}{\omega\sigma(\omega)}$$

Phys. Rev. B **67**, 241101 (2003)

$$\tau^{-1}(\omega) \equiv \mathrm{Re}\frac{\omega_p^2/4\pi}{\sigma(\omega)}$$

$$\sigma(\omega, T) = \frac{\omega_p^2 / 4\pi}{(\Gamma - i\omega)^{1-2\eta}(\Omega - i\omega)^{2\eta}}$$





$$\sigma(\omega) = \frac{C}{(\Gamma - i\omega)^{1-2\eta}}$$

$\eta=0.25$

Phenomenology of MnSi on a low energy scale
($T < 100$ K, $\omega < 20$ meV, magnetically ordered phase):

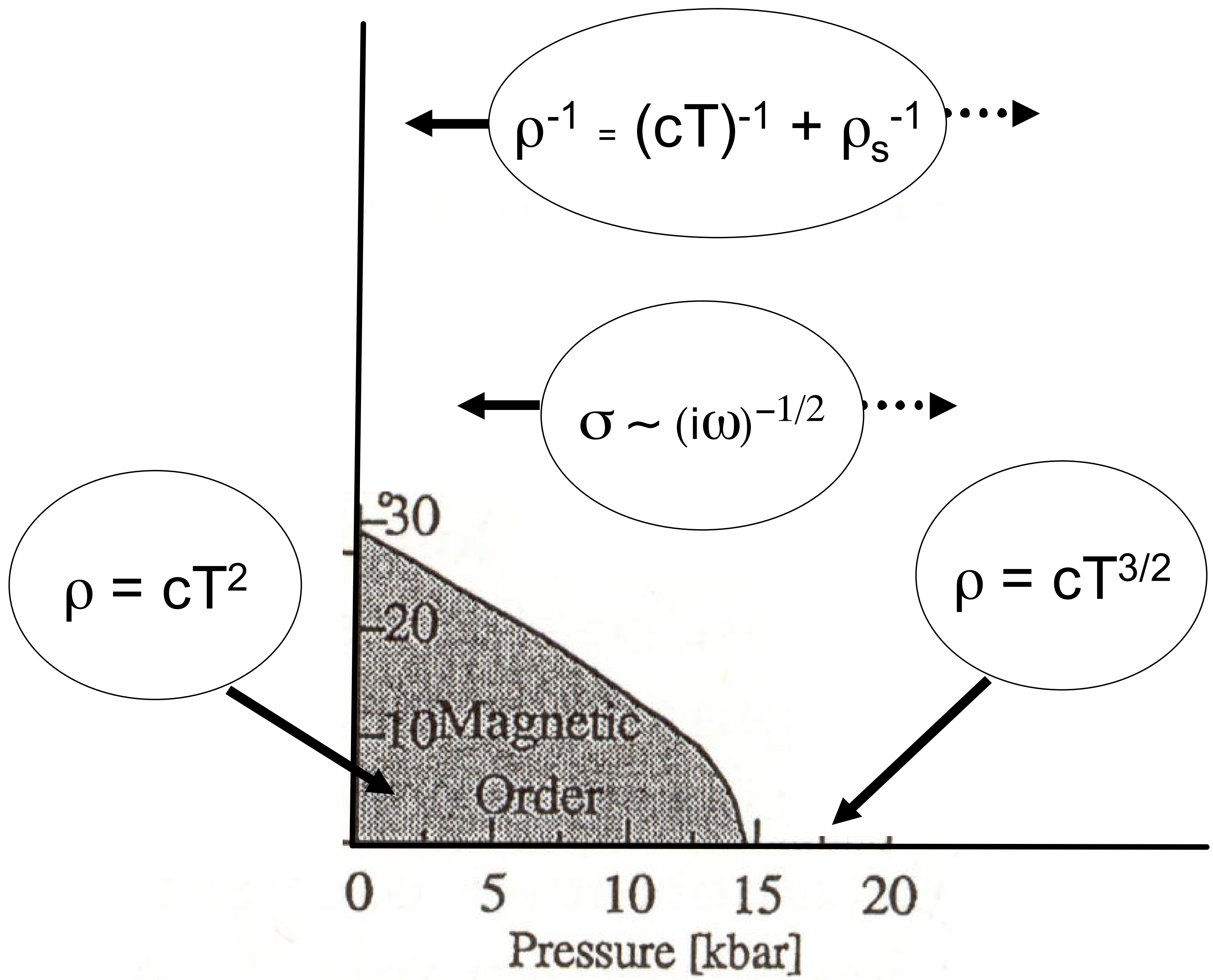
1) Band of itinerant charge carriers with mass $m^* \sim 10\, m_e$

2) Drude spectral weight: $\omega_p = 18700\ \text{cm}^{-1}$
Hence $Nm/m^* = 0.086$ per Mn atom

1) & 2) : Each Mn atom contributes 1 charge carrier.

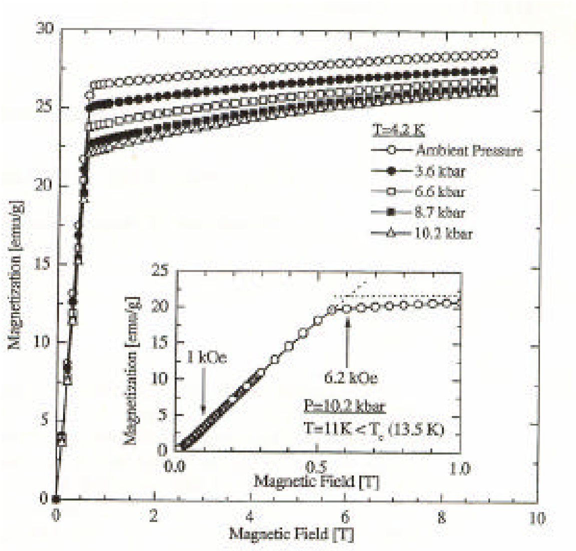
Strong inelastic scattering of the charge carriers
(and weak residual scattering, clean limit!)
Helimagnetic phase: $1/\tau \sim \omega, T^2$
Paramagnetic phase: $1/\tau \sim \omega^2, T$
$\rho = \alpha T - \rho_0$ with $\rho_0 \sim 0$

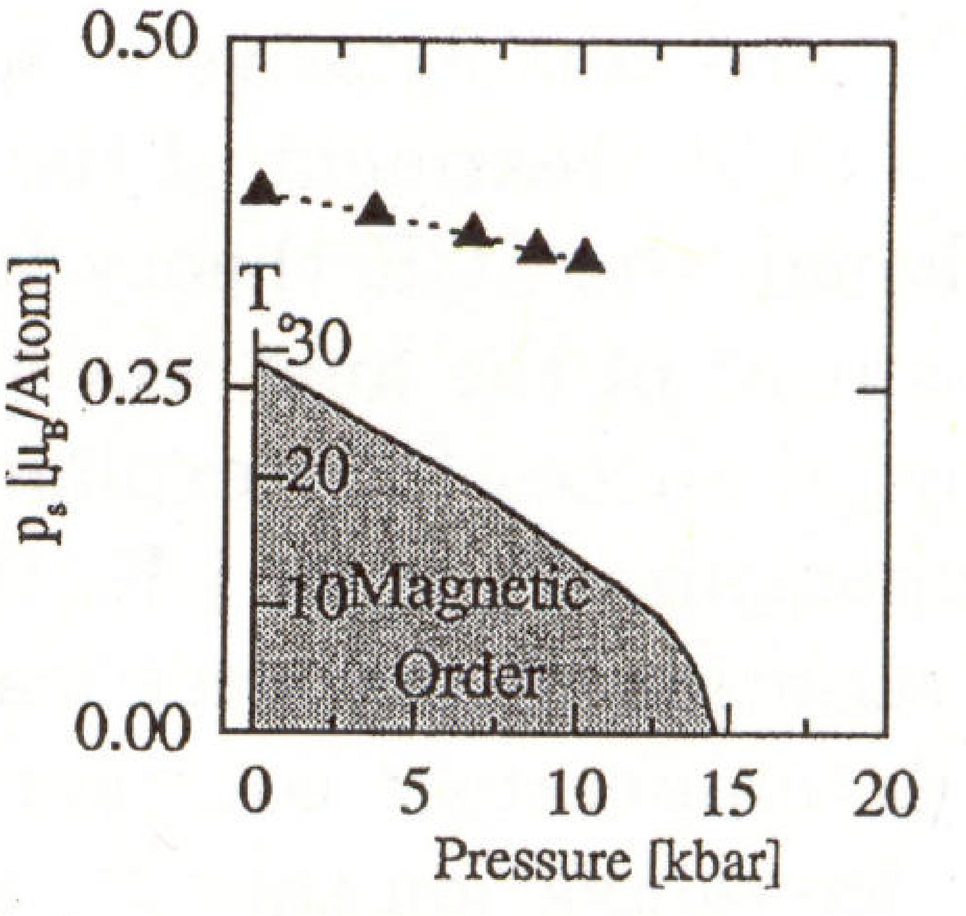
$$\sigma(\omega,T) = \frac{\omega_p^2 / 4\pi}{(\Gamma - i\omega)^{1/2}(\Omega - i\omega)^{1/2}}$$

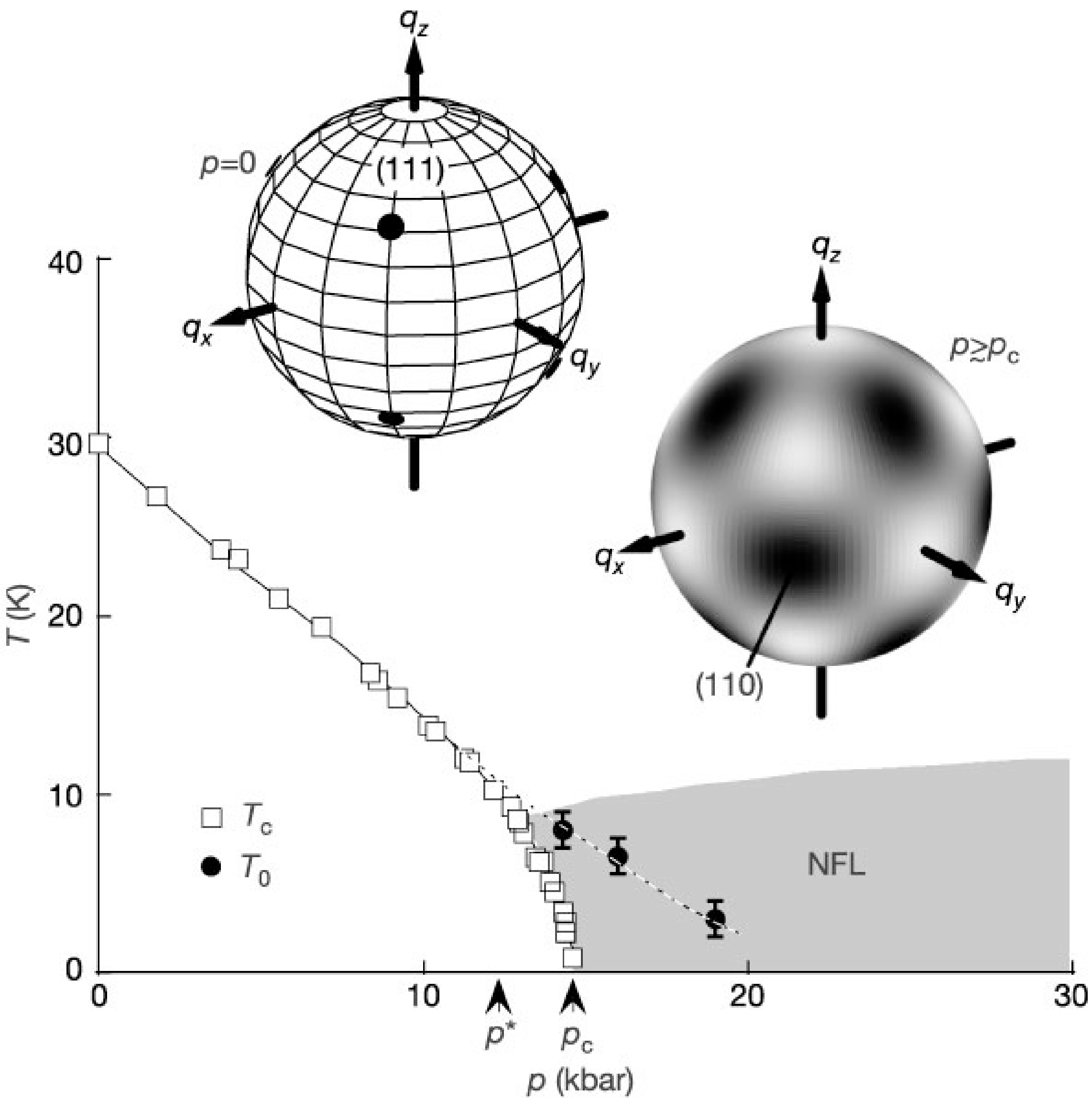

ρ^-1 = (cT)^-1 + ρ_s^-1
σ ~ (iω)^−1/2
ρ = cT^2
ρ = cT^3/2
30
20
10
Magnetic
Order
0
5
10
15
20
Pressure [kbar]

Saturation Magnetization

Thessieu, J. Phys. Soc Jpn 67, 3605 (1998)

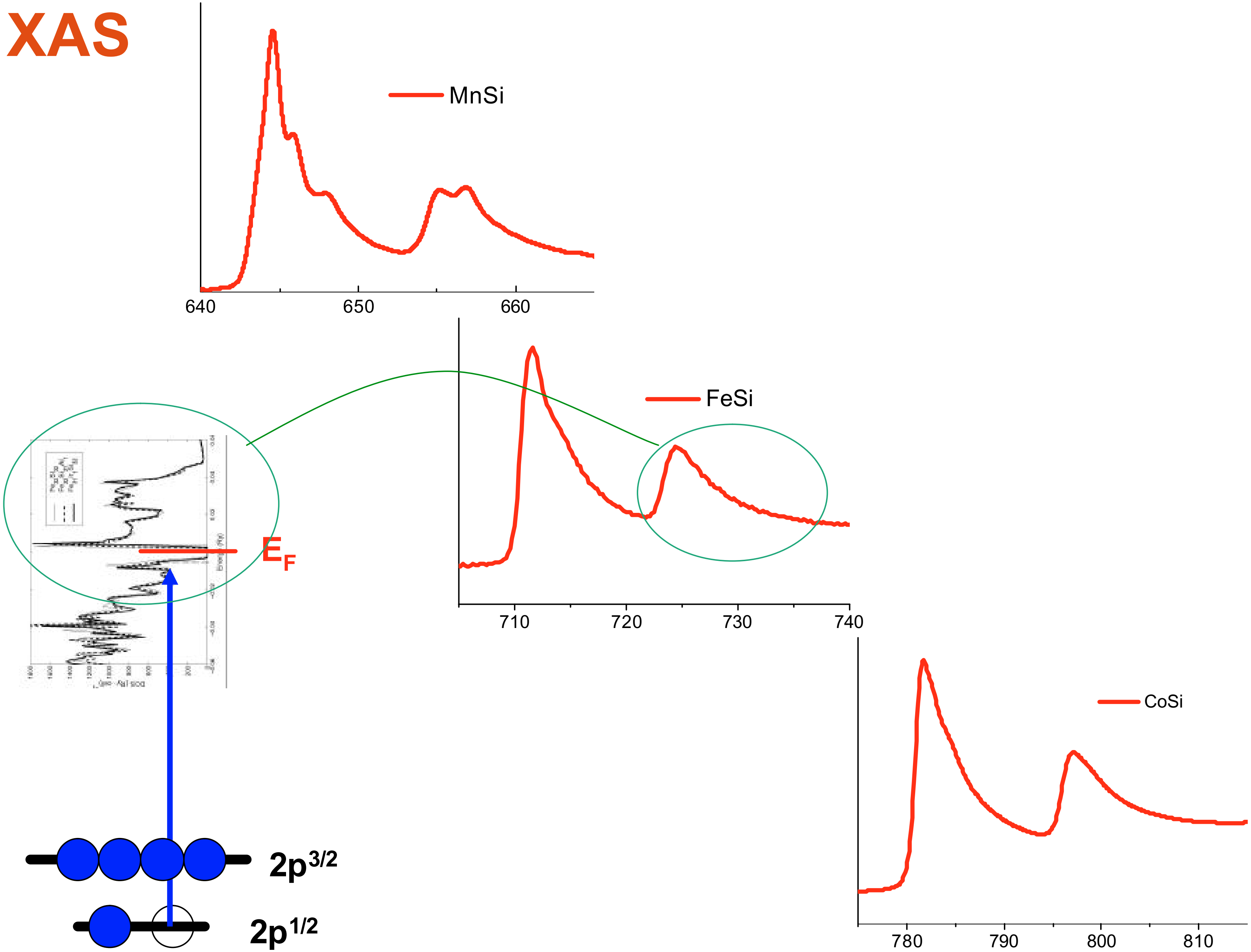






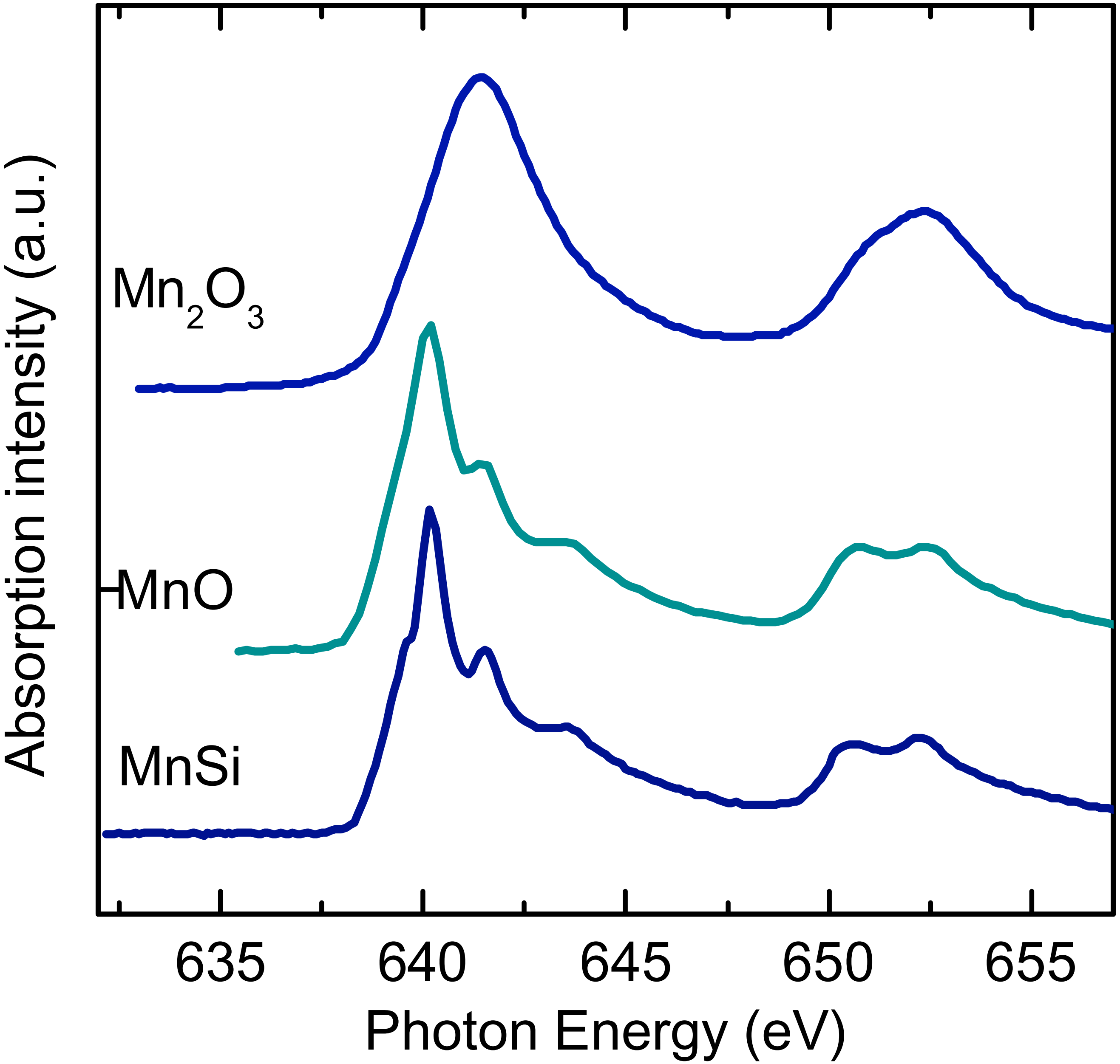
C. Pfleiderer et al, *Nature* **427**, 227 - 231 (15 Jan 2004)

XAS



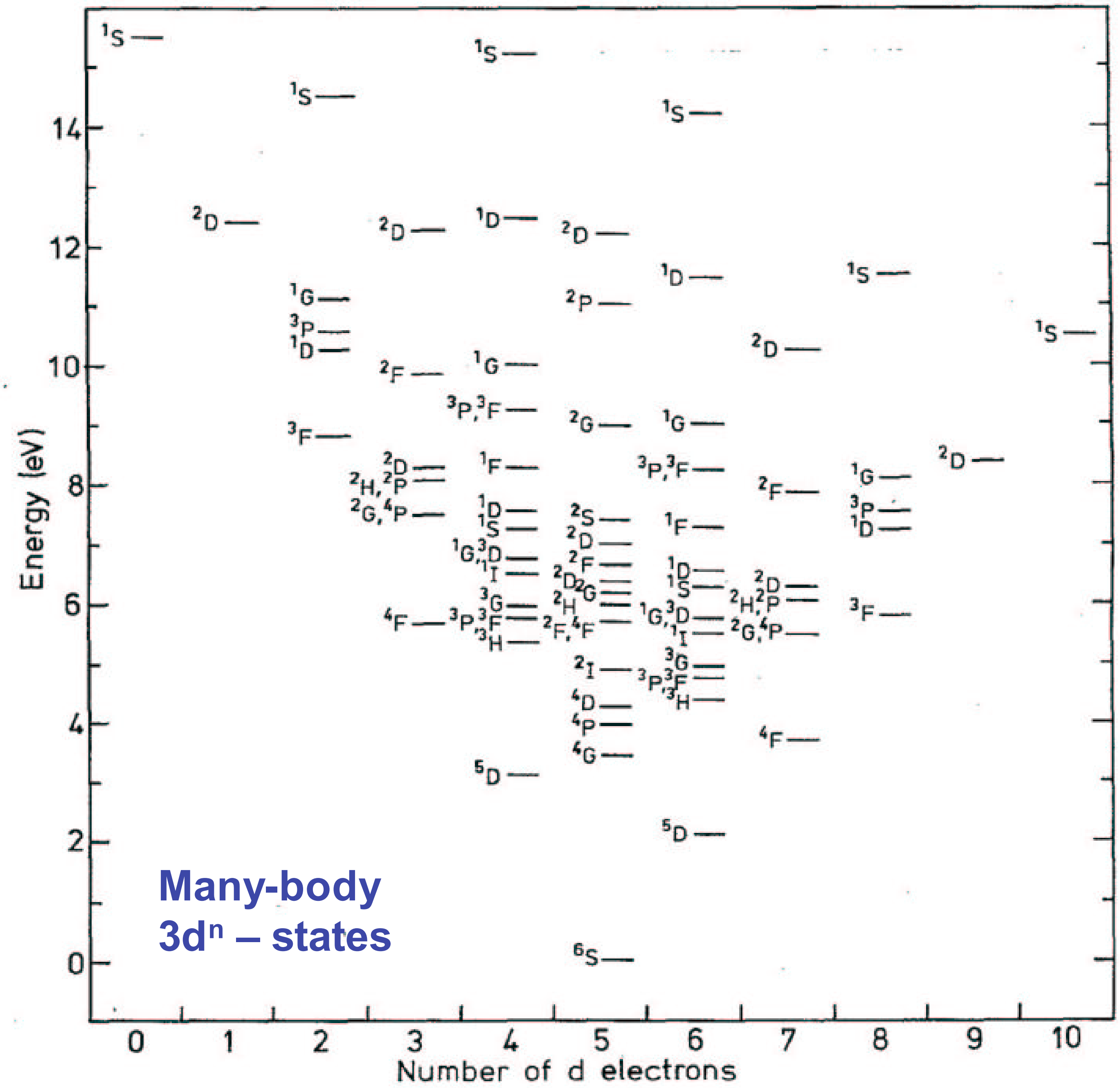
MnSi
640
650
660
FeSi
710
720
730
740
CoSi
780
790
800
810
E_F
2p^{3/2}
2p^{1/2}

XAS

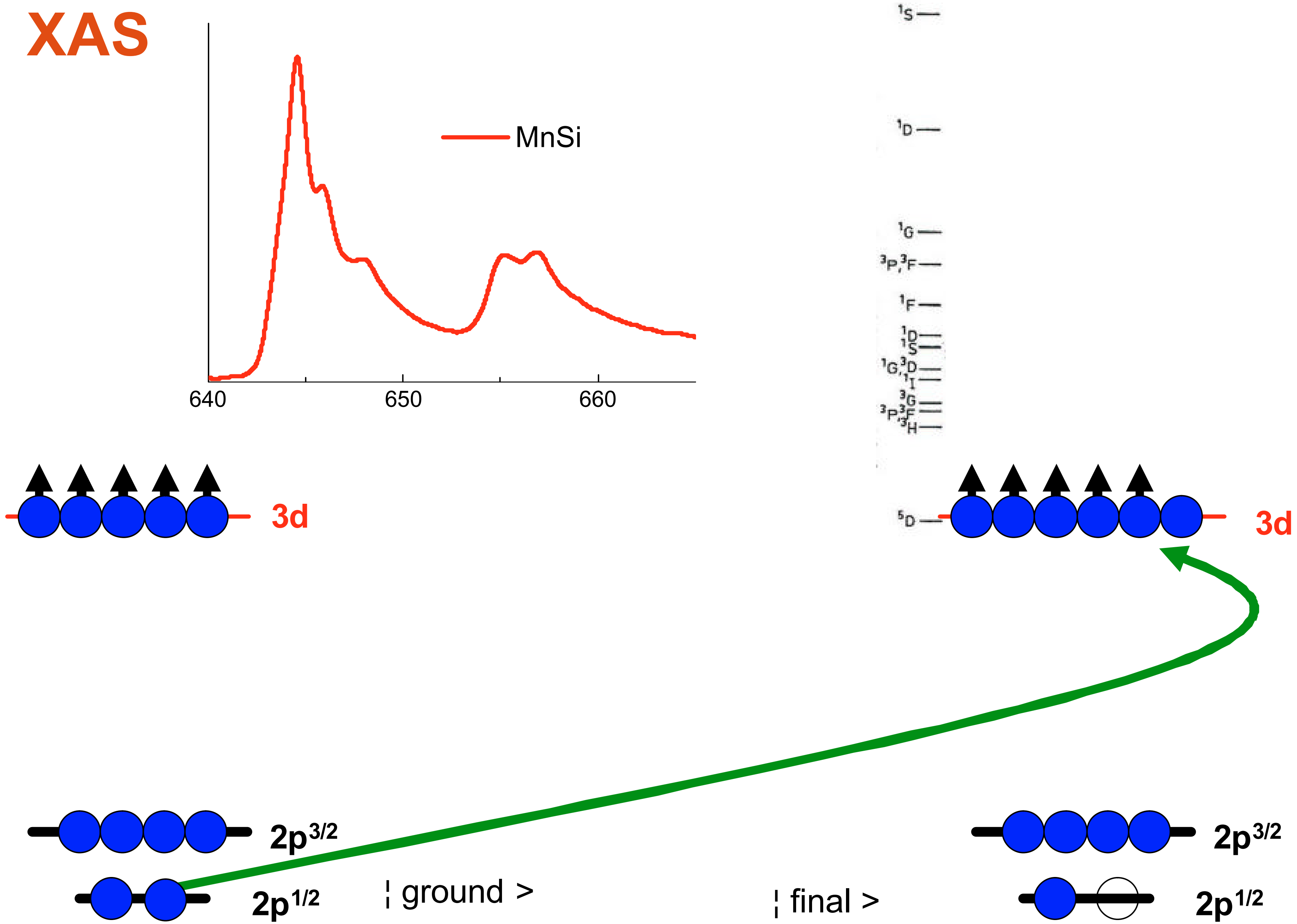


Mn2O3
MnO
MnSi
Absorption intensity (a.u.)
635
640
645
650
655
Photon Energy (eV)

Many-body $3d^n$ – states

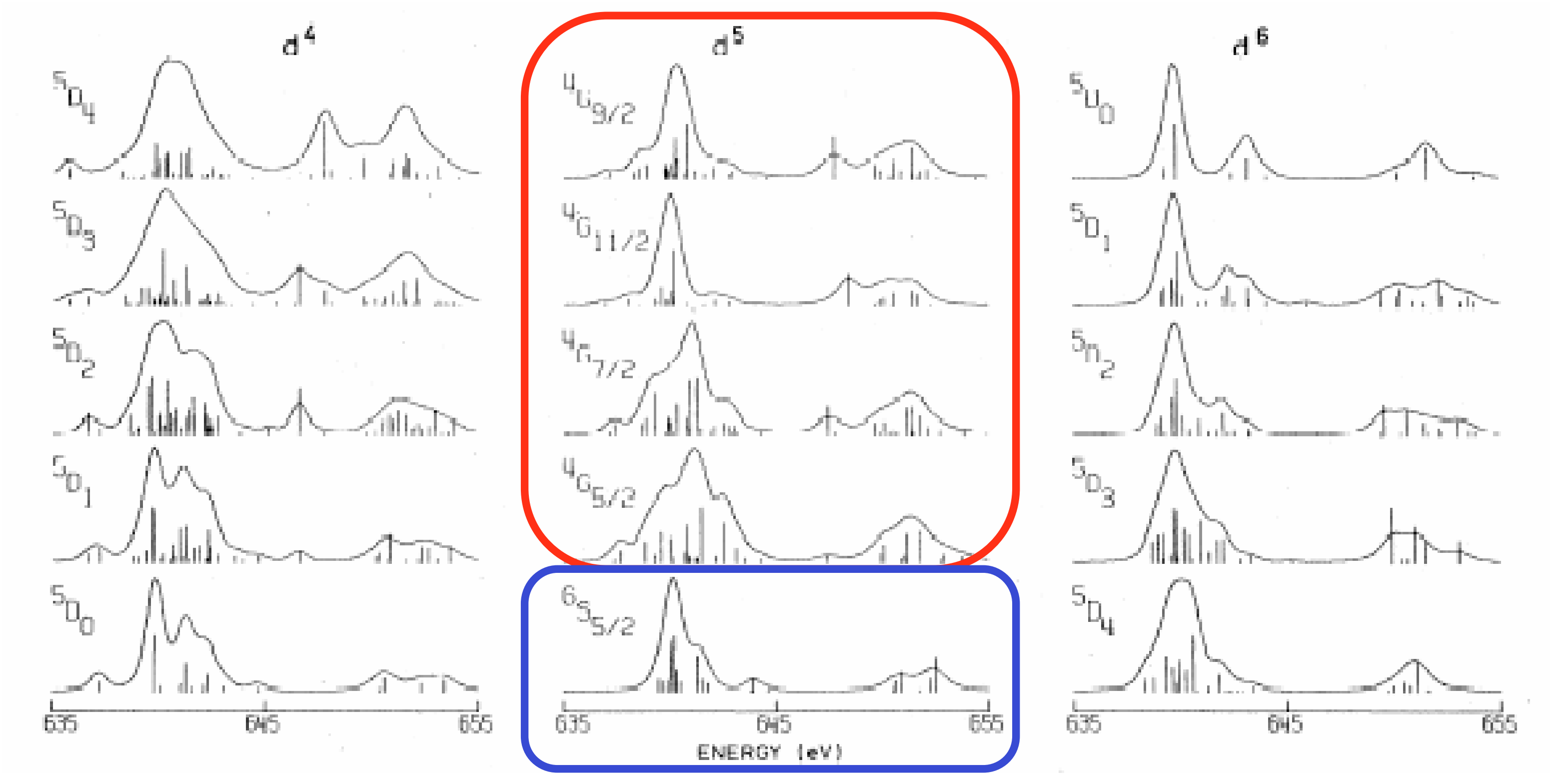


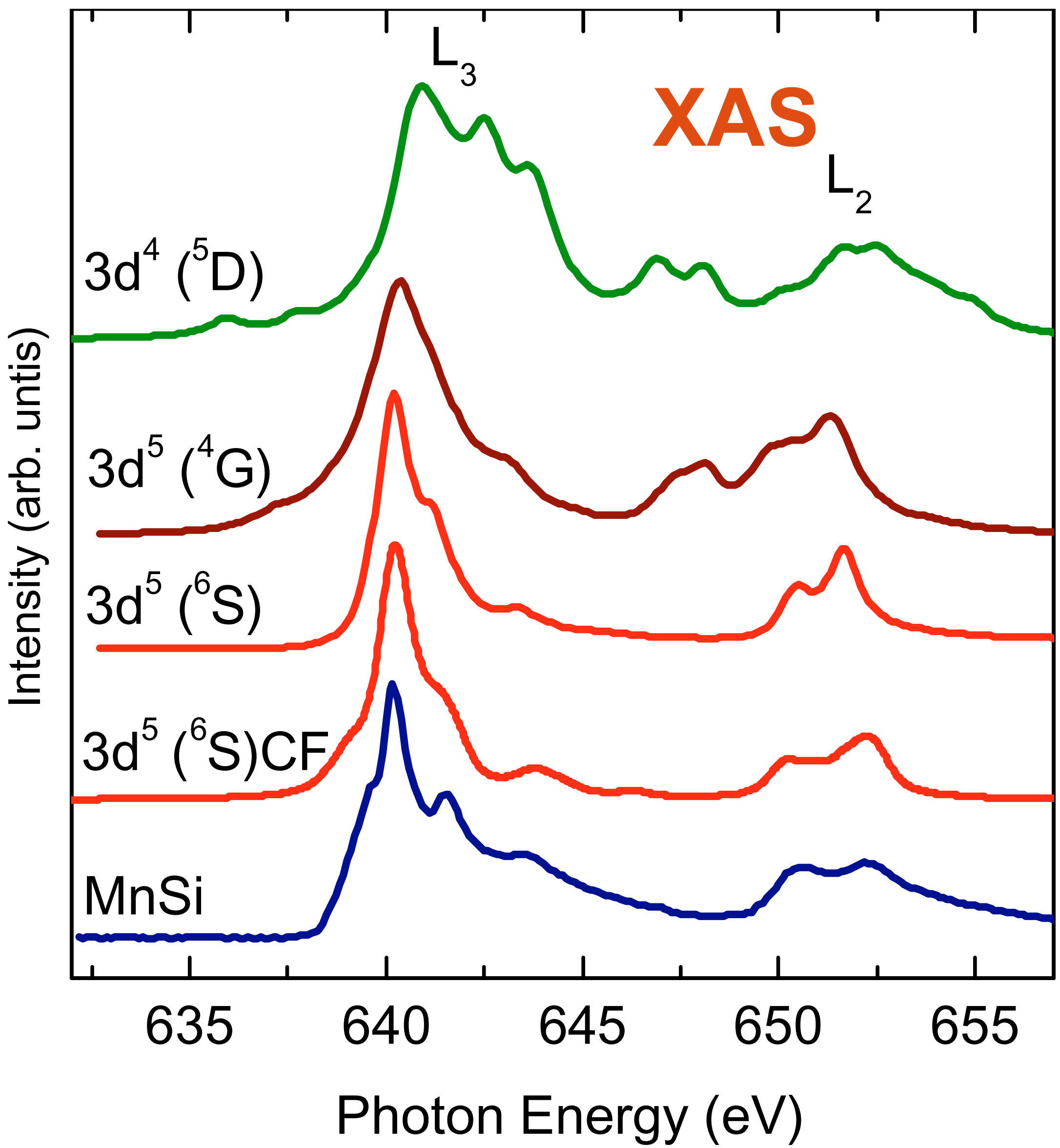
XAS



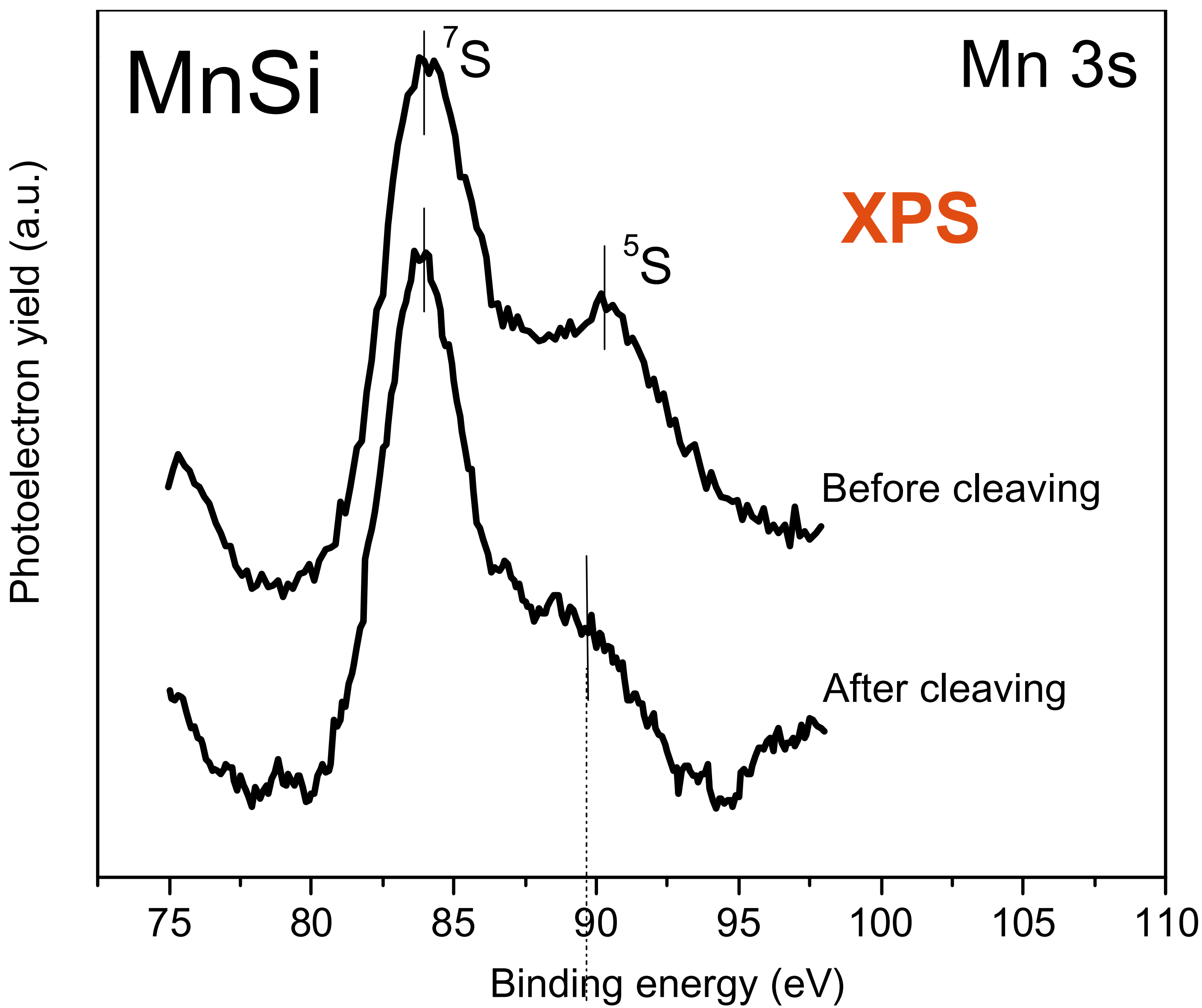
XAS

Some theoretical calculations for different ground states

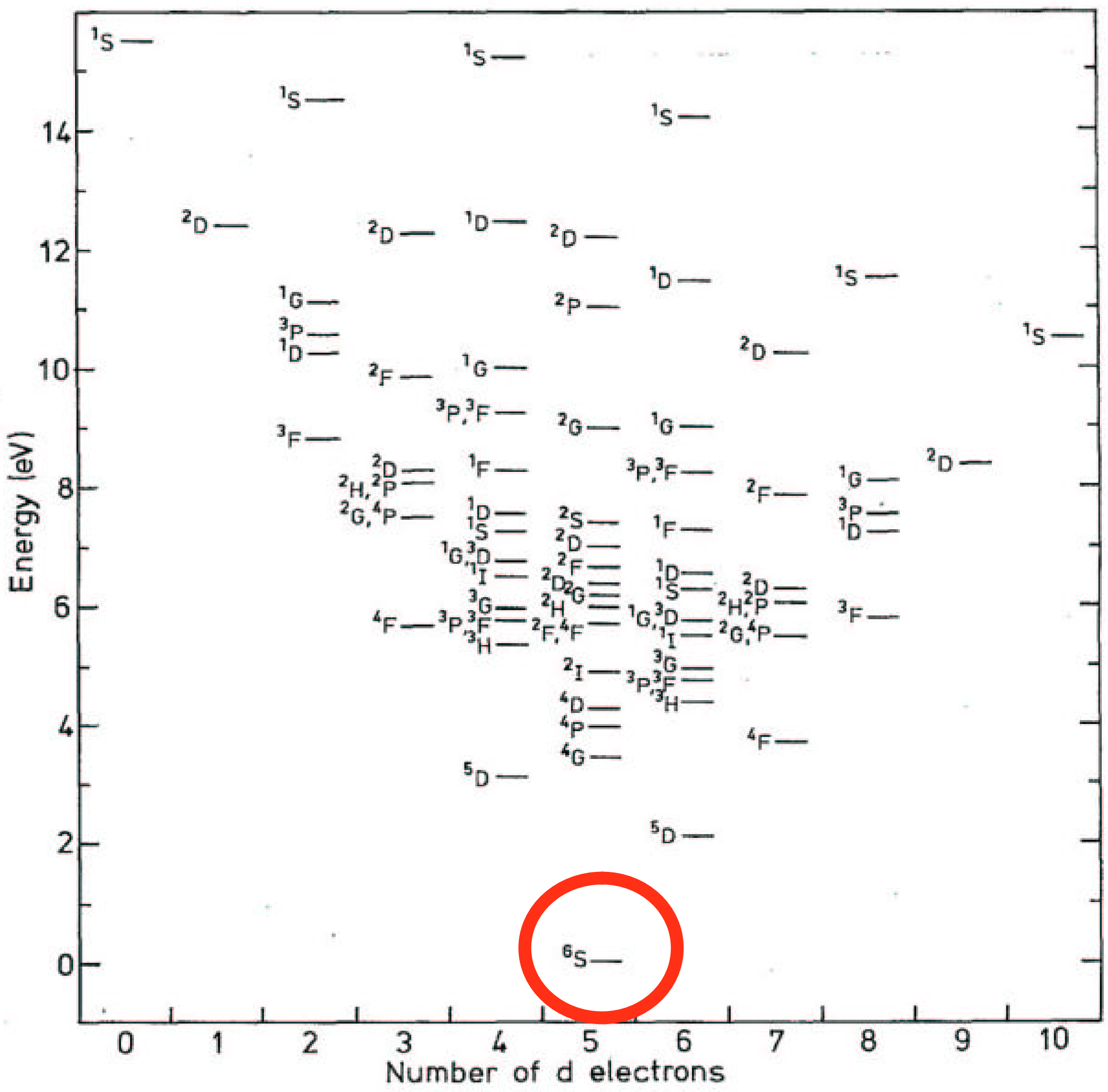




L3
XAS
L2
3d4 (5D)
3d5 (4G)
3d5 (6S)
3d5 (6S)CF
MnSi
Intensity (arb. untis)
635
640
645
650
655
Photon Energy (eV)

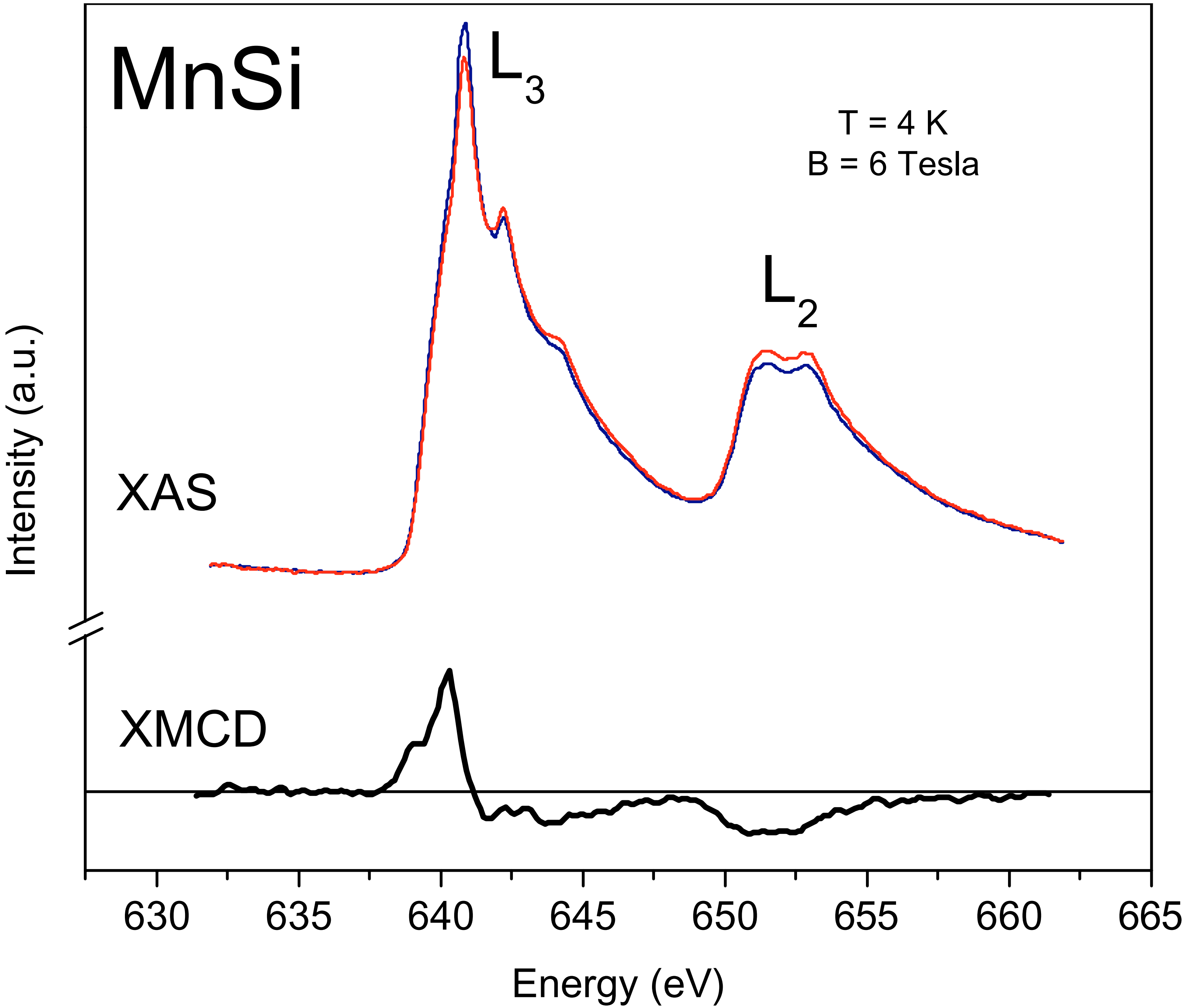


MnSi
Mn 3s
XPS
^{7}S
^{5}S
Before cleaving
After cleaving
Photoelectron yield (a.u.)
Binding energy (eV)
75
80
85
90
95
100
105
110



5 localized d-electrons per Mn-atom with parallel spins

Total Spin = 5/2
Total L = 0


MnSi
L_3
L_2
T = 4 K
B = 6 Tesla
XAS
XMCD
Intensity (a.u.)
630
635
640
645
650
655
660
665
Energy (eV)

•Saturation moment $T<T_C$: 0.4 μ_B

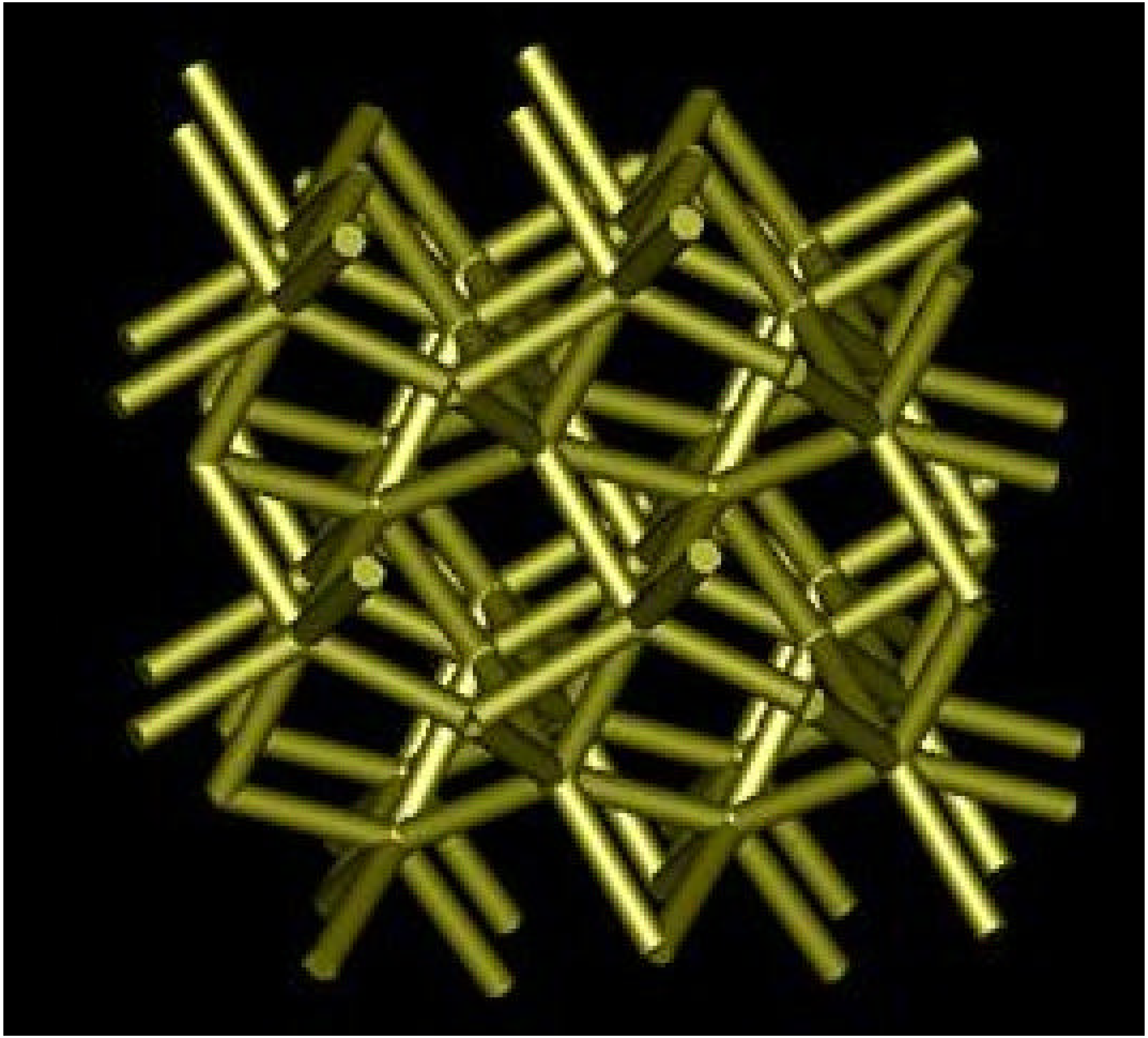
•Curie-Weiss moment $T>T_C$: 2.5 μ_B

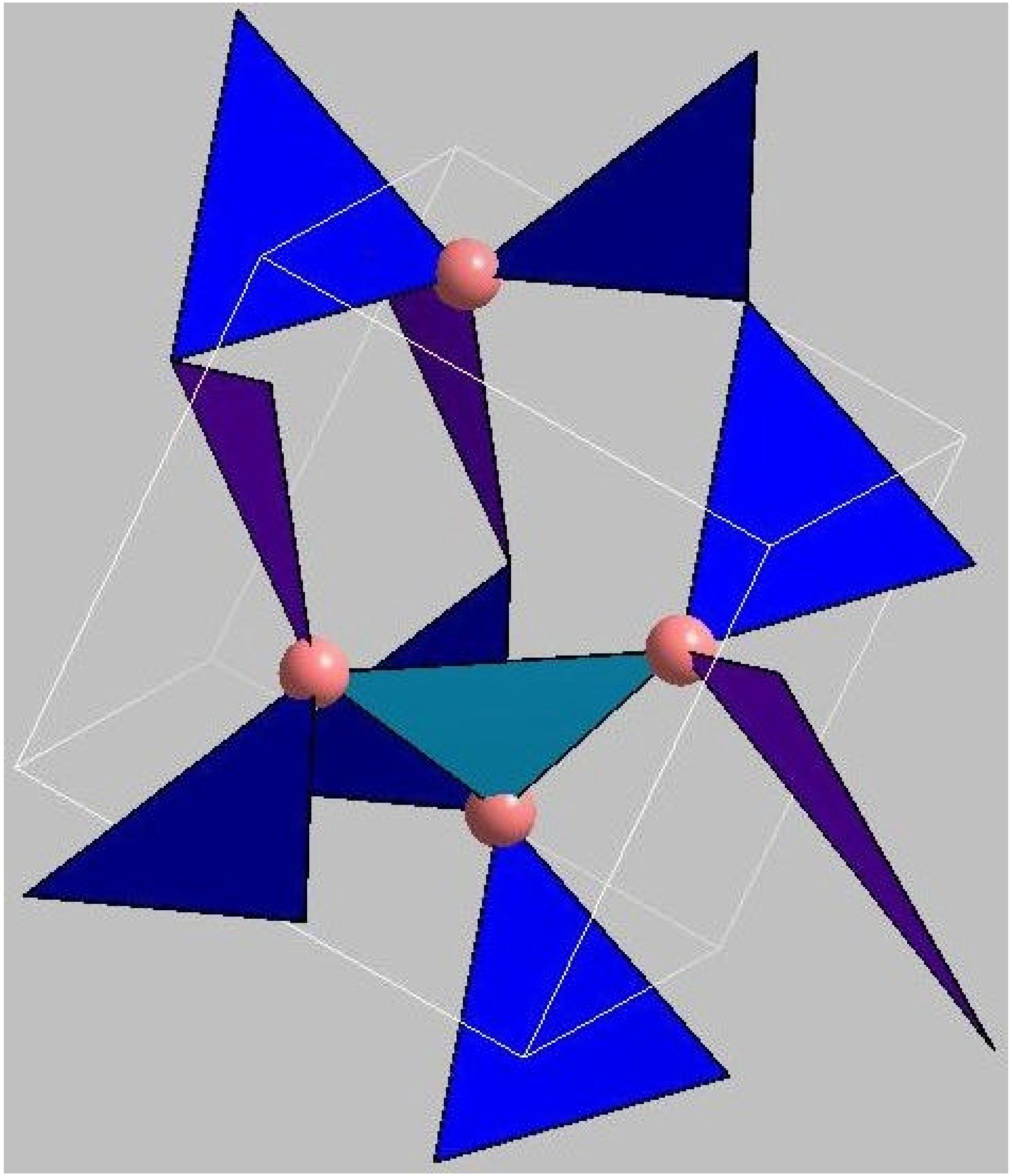
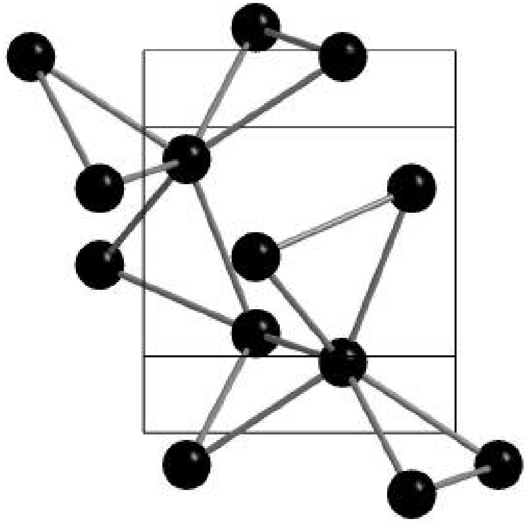
•Local magnetic structure of MnSi is $d^5(^6S)$: 6 μ_B

-5 localized d-electrons per Mn-atom

-Total Spin = 5/2

-Total L = 0



Summary FeSi:

•Semiconductor gap closes at ~ 100 K. Above 100 K it is a bad metal.

•Optical spectral weight removed from the gap is not recovered upto 4 eV.

•The gap gets filled when Fe is partially substituted with Co.

Summary MnSi:

• 1 heavy electron (~10 me) per Mn atom.

• $T > T_C$: ?/t ~7 kBT Spin-flip scattering off local moments?

•Strong local $d^5(^6S)$ spin-correlations on the Mn-sites

•3D triangular Mn sublattice: Possible role of magnetic frustration