Optical study on CuxTiSe2

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Outline

- Structure in dichalcogenides
  1 T and 2 H phases
- Coexistence and competition between CDW and SC

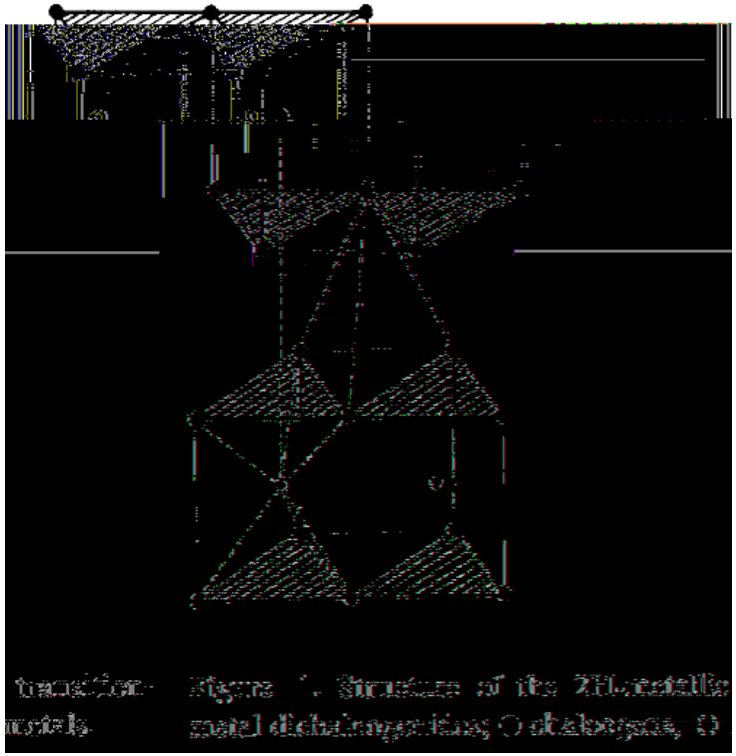
- Parent compound 1T-TiSe2
  semimetal or semiconductor?
  mechanism of CDW transition:
  excitonic or others

- Cu-doped compound CuxTiSe2
  evolution
  x=0.07, anomalous metallic state

2H structure

a=3.314 A, c=12.090 A

Space group *P*6/mmc

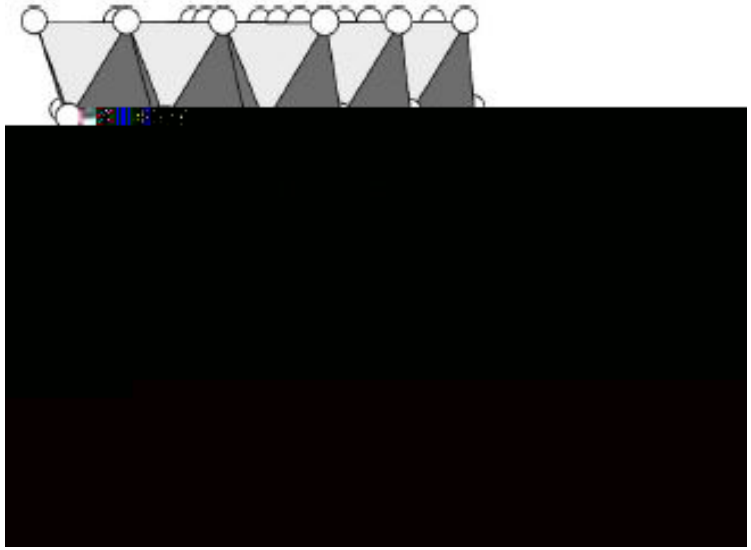


2H-TaS_2

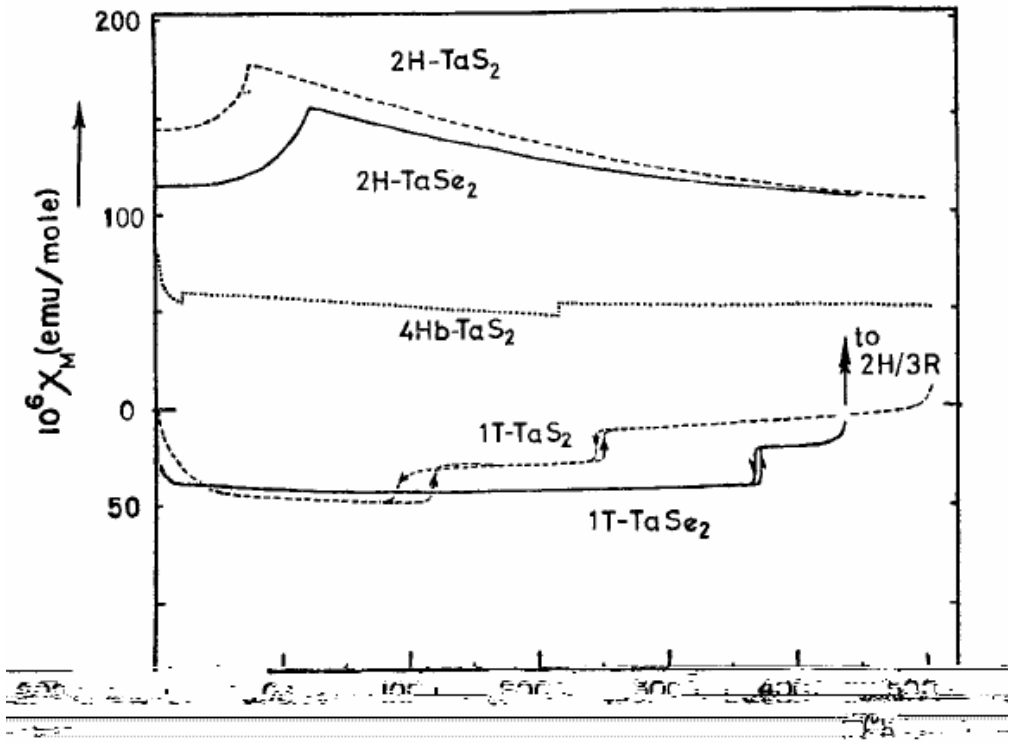
1T structure

A=3.364 A c=5.897 A

Space group: *P*3m1



1T-TaS_2

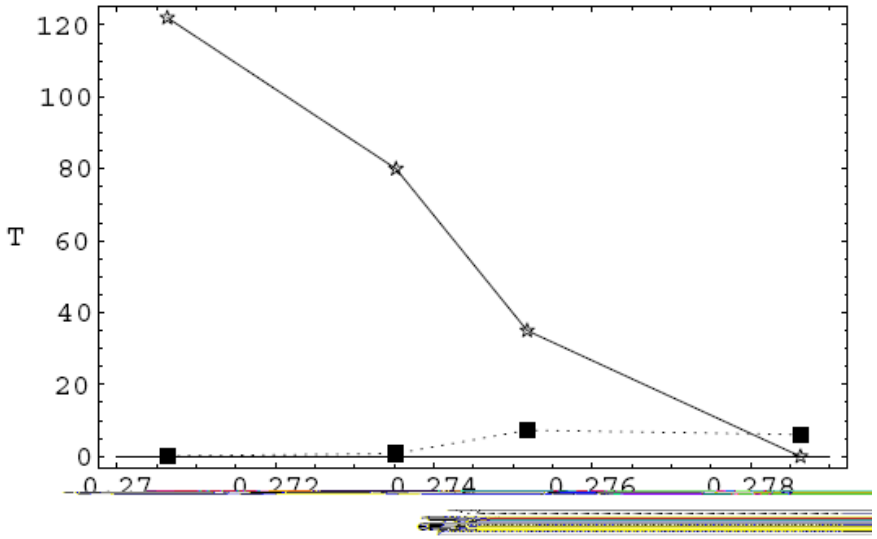

200
100
0
50
$10^6\chi_M$(emu/mole)
2H-TaS$_2$
2H-TaSe$_2$
4Hb-TaS$_2$
to
2H/3R
1T-TaS$_2$
1T-TaSe$_2$

Coexistence and competition between CDW and SC:

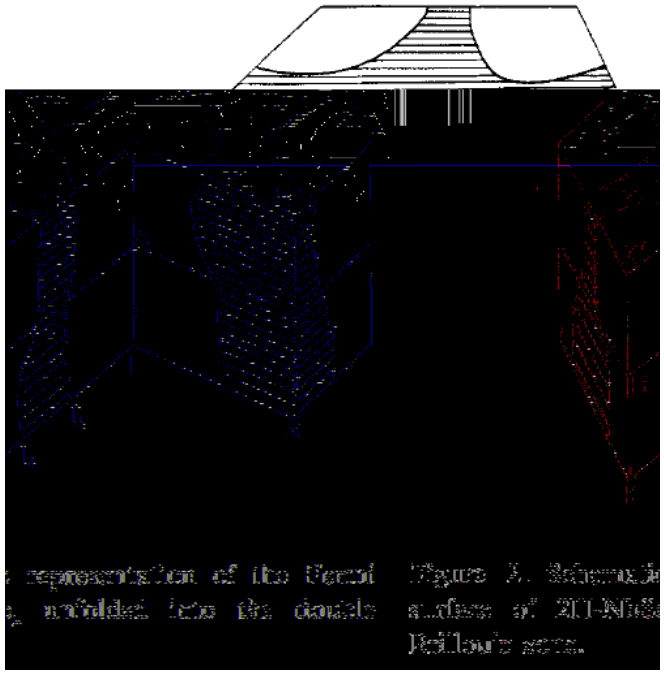
	2H-TaSe2,	2H-TaS2,	2H-NbSe2,	2H-NbS2
T_{CDW}:	122 K (90 K),	75 K,	35 K,	0 K
T_{sc}:	0.14 K,	0.7 K,	7.2 K,	6 K

Na-intercalated 2H-TaS2:

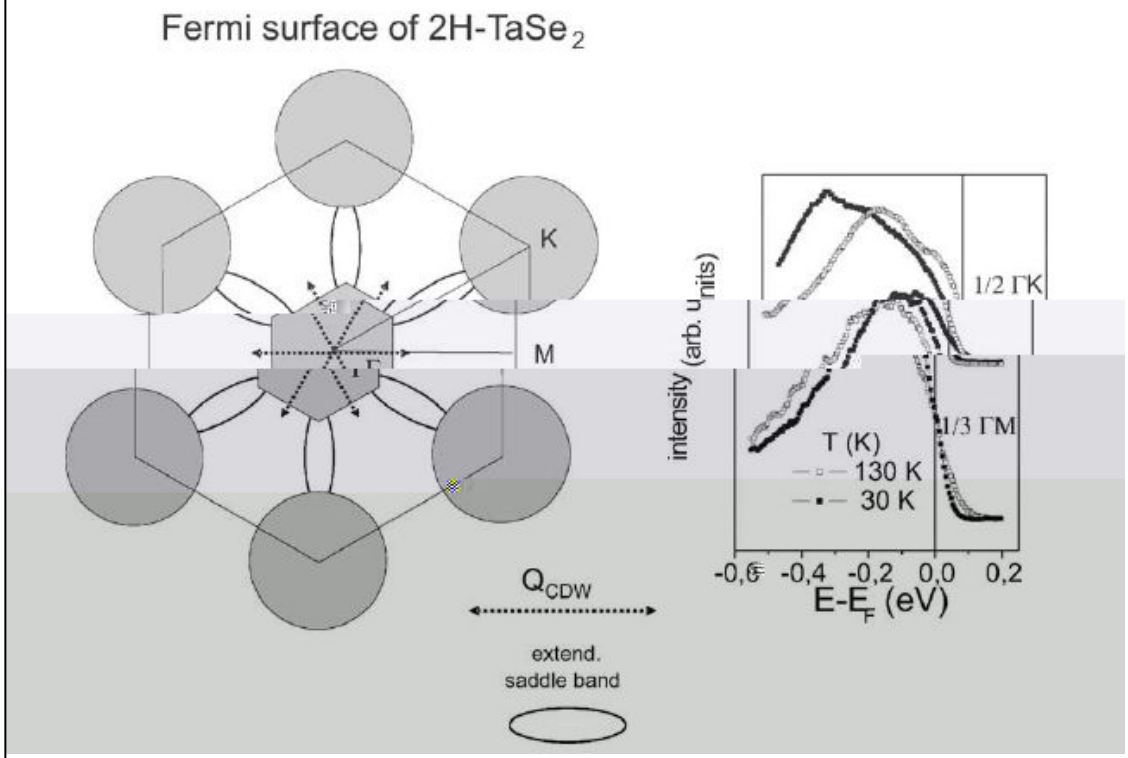
CDW suppressed, but SC increases



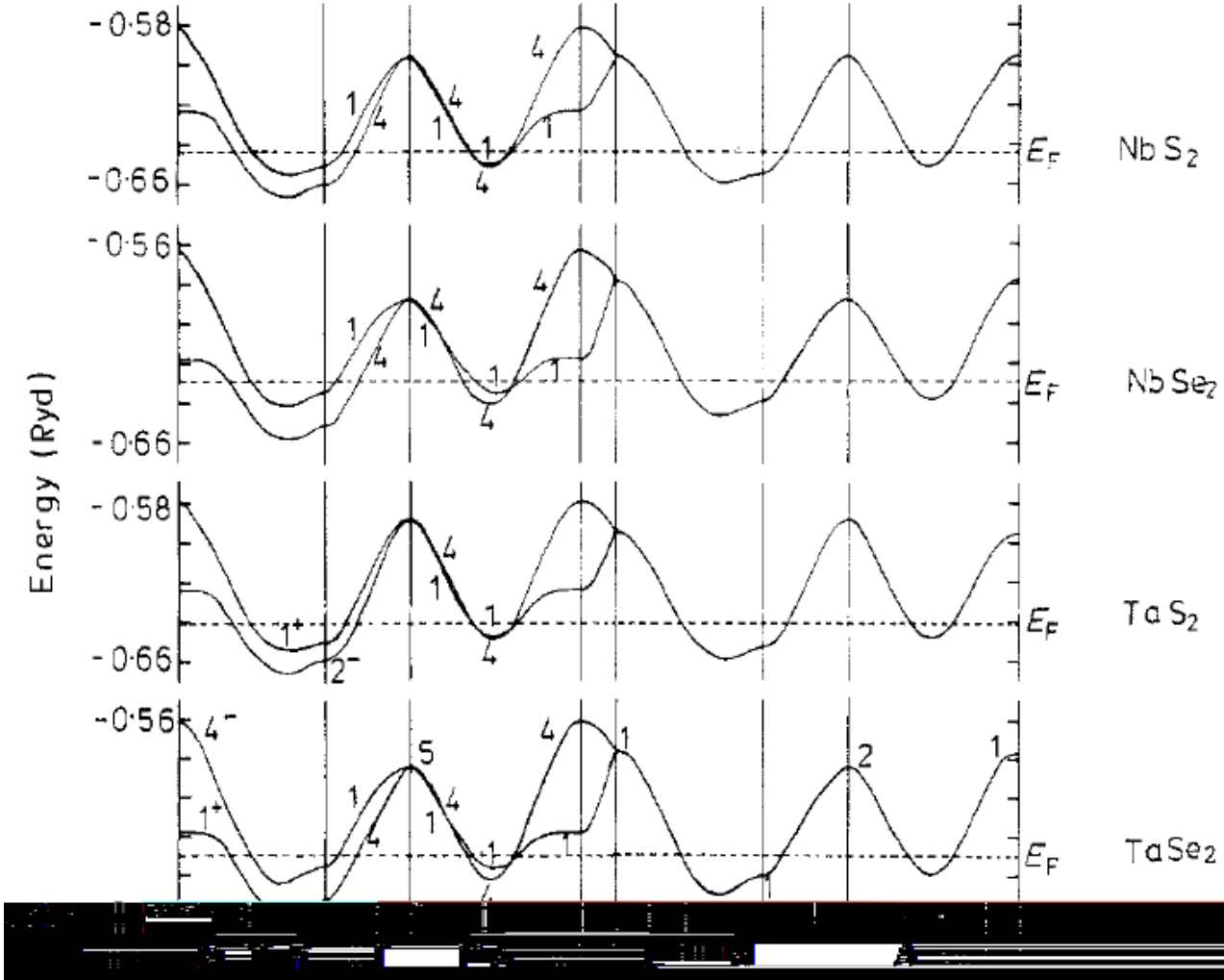
A. H. Castro Neto, PRL (01)



O. Seifarth et al. / Journal of Electron Spectroscopy and Related Phenomena 137–140 (2004) 675–679



CDW wave vector is 1/3**b** (2/3Γ**M**) regardless of doping, or element.

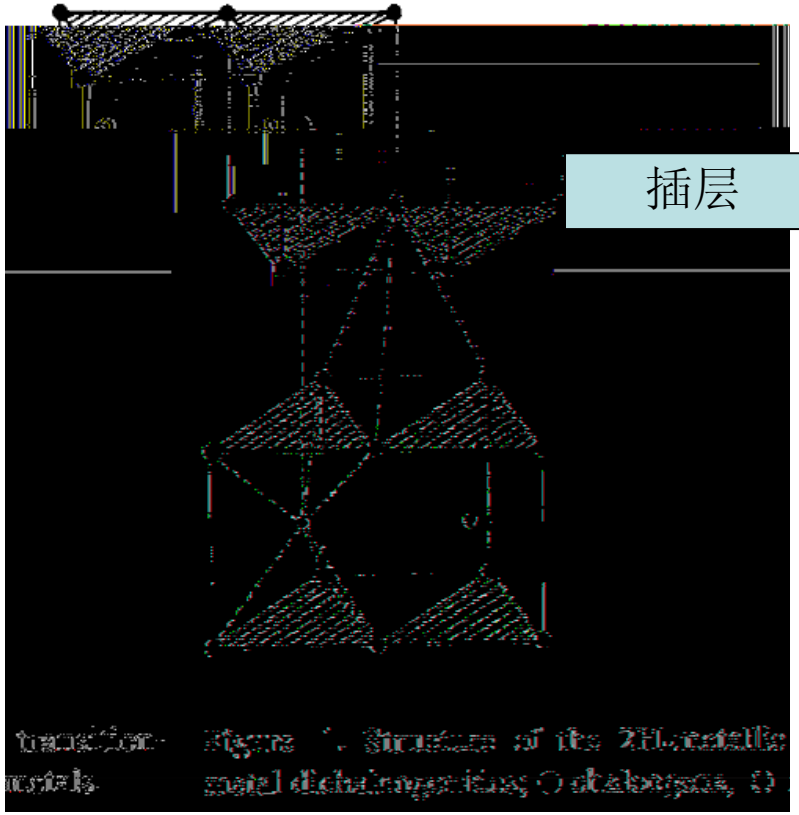


4. Lowest 6 sub-bands (d_{z^2} at Γ) for the four 2H-type dichalcogenides. The small [illegible] between the Nb and Ta compounds may be increased by relativistic corrections. [illegible]

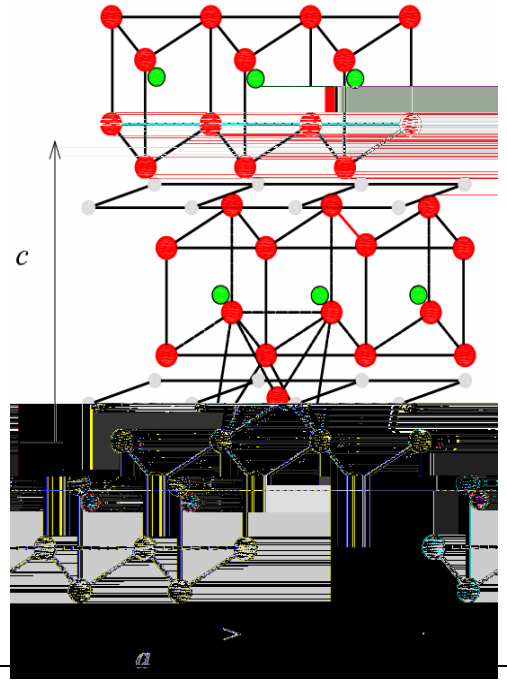
Fermi surfaces and band structures of the 2H metallic transition-metal dichalcogenides

G Wexler and A M Woolley
Cavendish Laboratory, Madingley Road, Cambridge, CB3 0HE, England

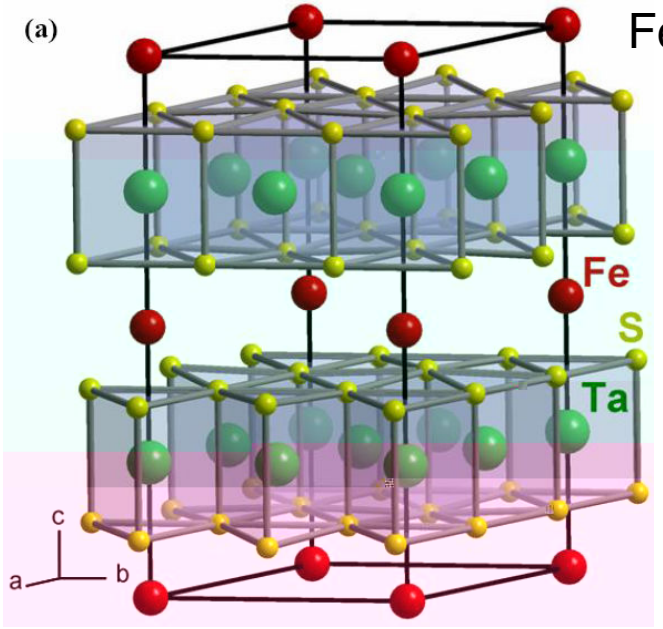
Received 8 August 1975



插层



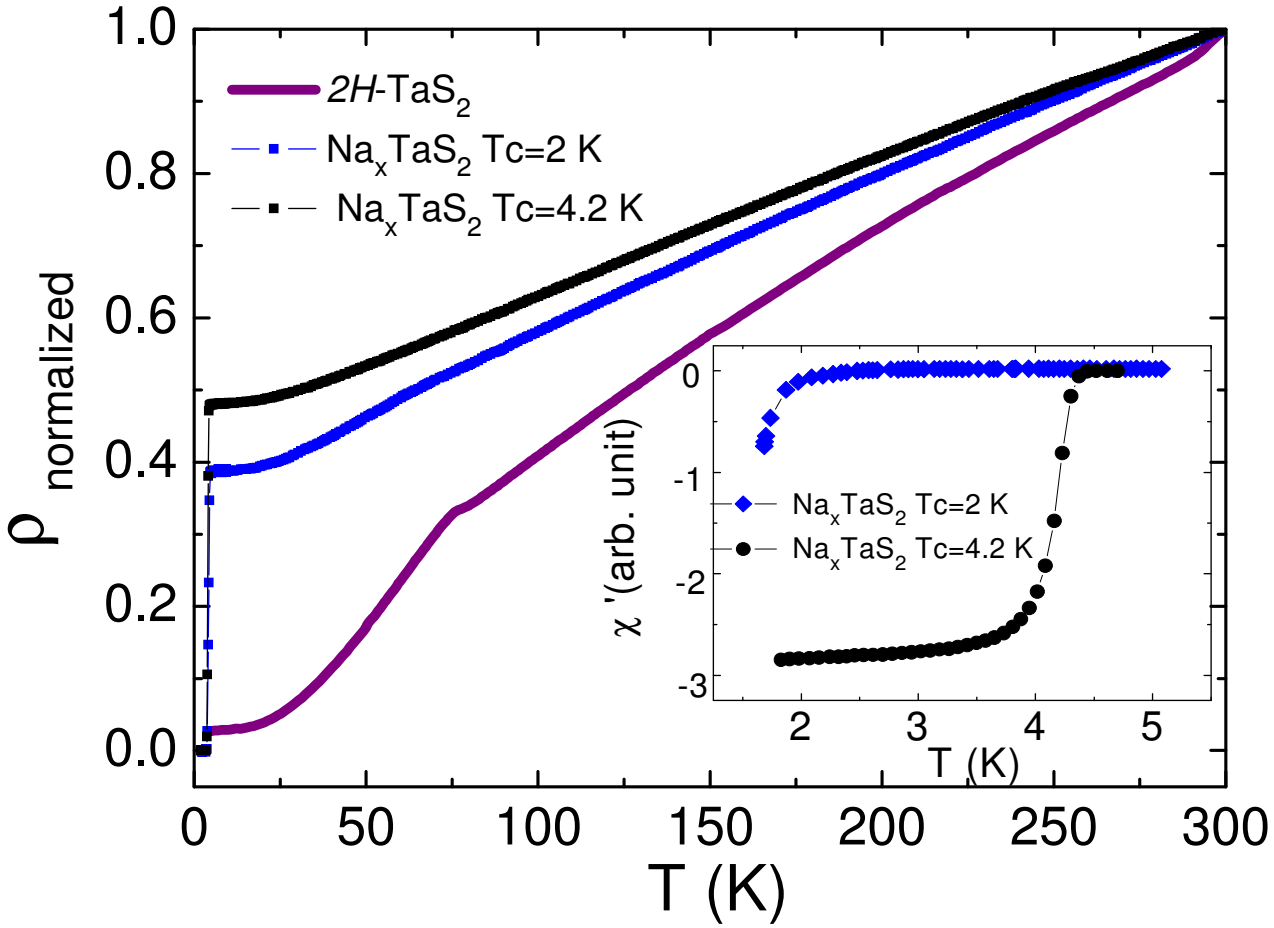
LixNbO2

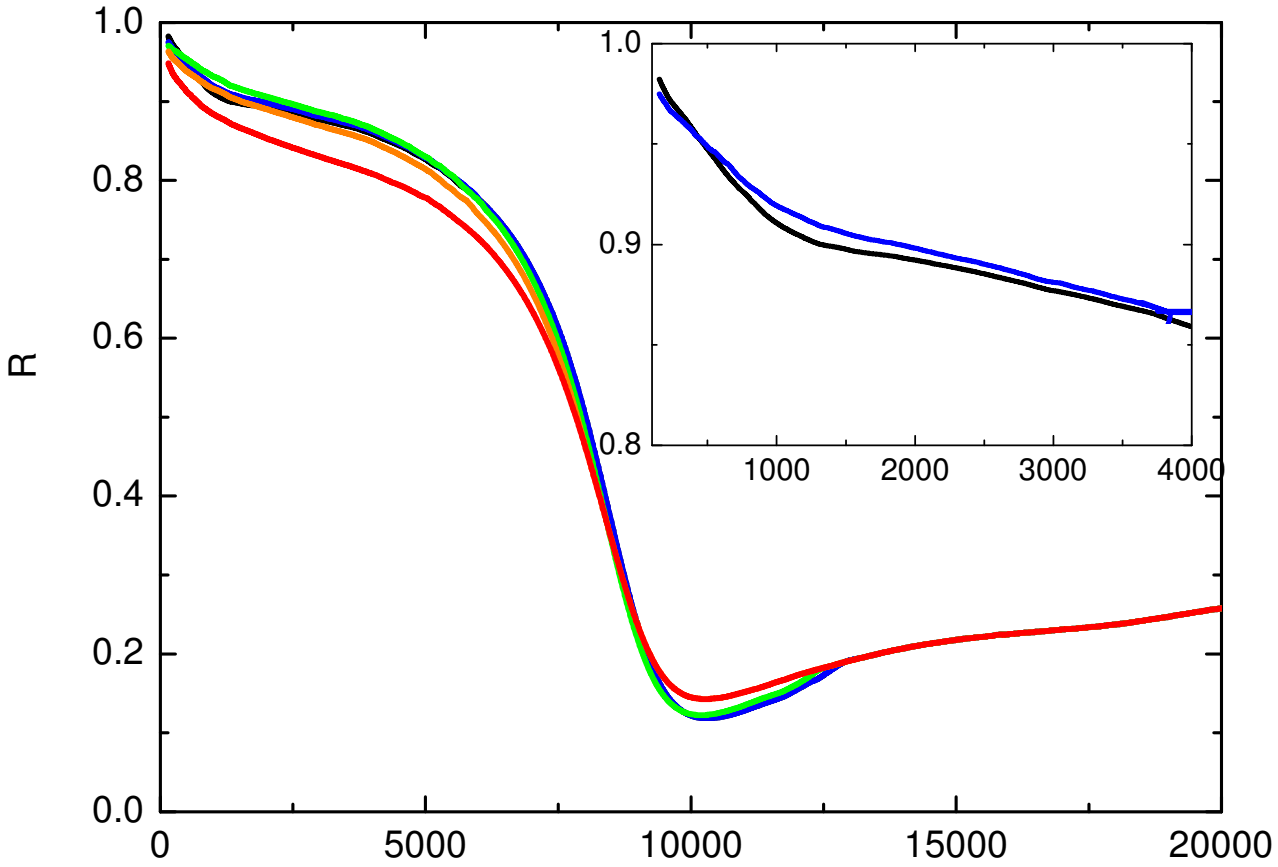


Fe1/4TaS2

E. Morosan et al. cond-mat/0701311

2H-NaxTaS2


1.0
0.8
0.6
0.4
0.2
0.0
ρ normalized
2H-TaS2
NaxTaS2 Tc=2 K
NaxTaS2 Tc=4.2 K
0
50
100
150
200
250
300
T (K)
0
-1
-2
-3
χ '(arb. unit)
NaxTaS2 Tc=2 K
NaxTaS2 Tc=4.2 K
2
3
4
5
T (K)


R
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0
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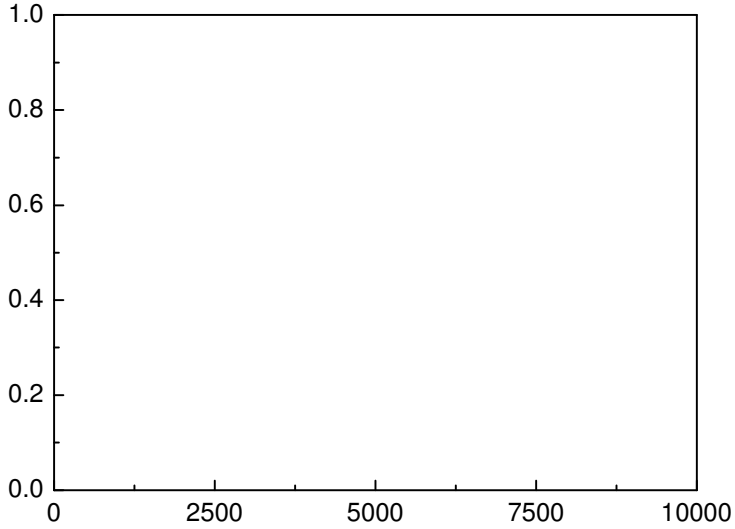
10000
15000
20000
1.0
0.9
0.8
1000
2000
3000
4000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0.2
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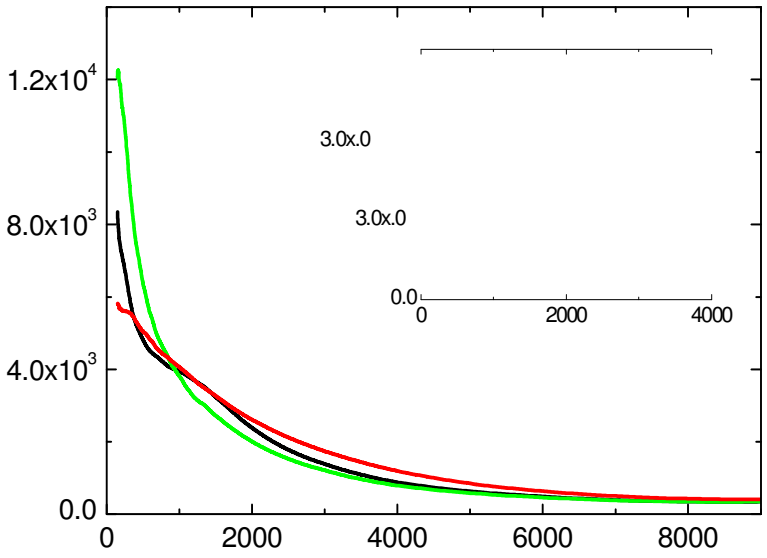
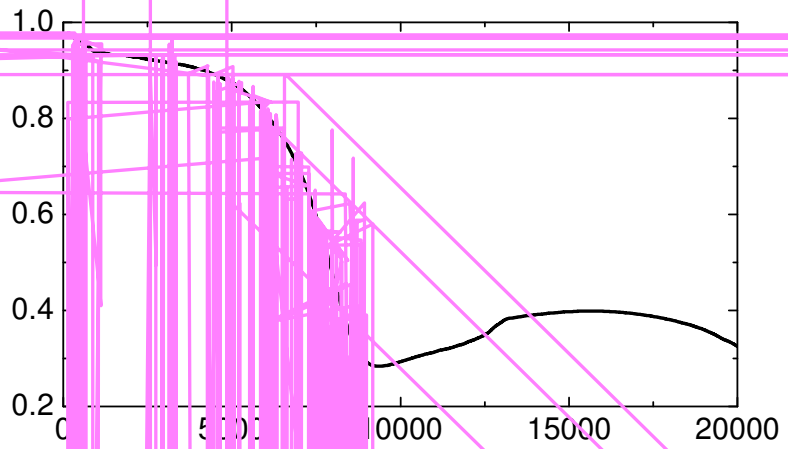
7500
10000


1.2x10^4
8.0x10^3
4.0x10^3
0.0
0
2000
4000
6000
8000
3.0x.0
3.0x.0
0.0
0
2000
4000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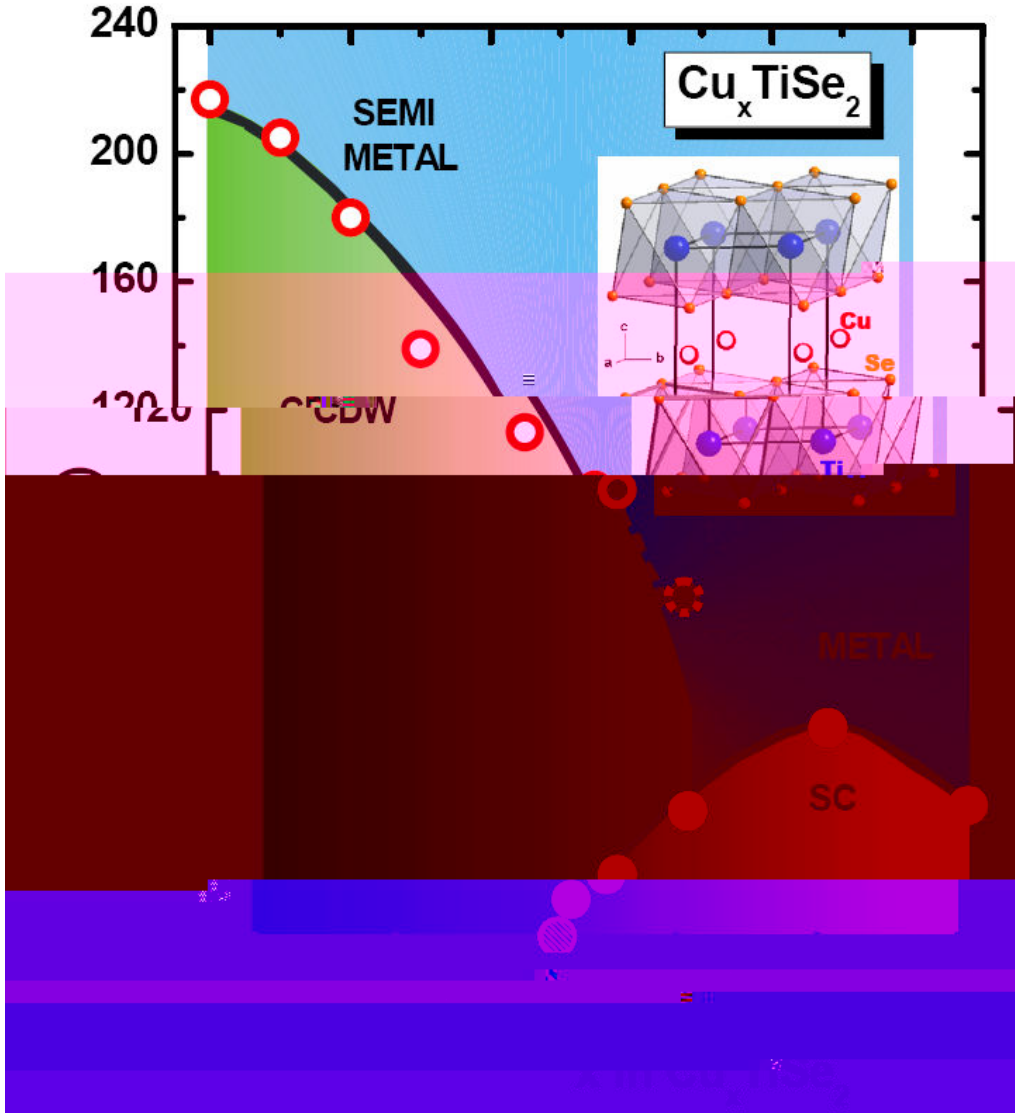
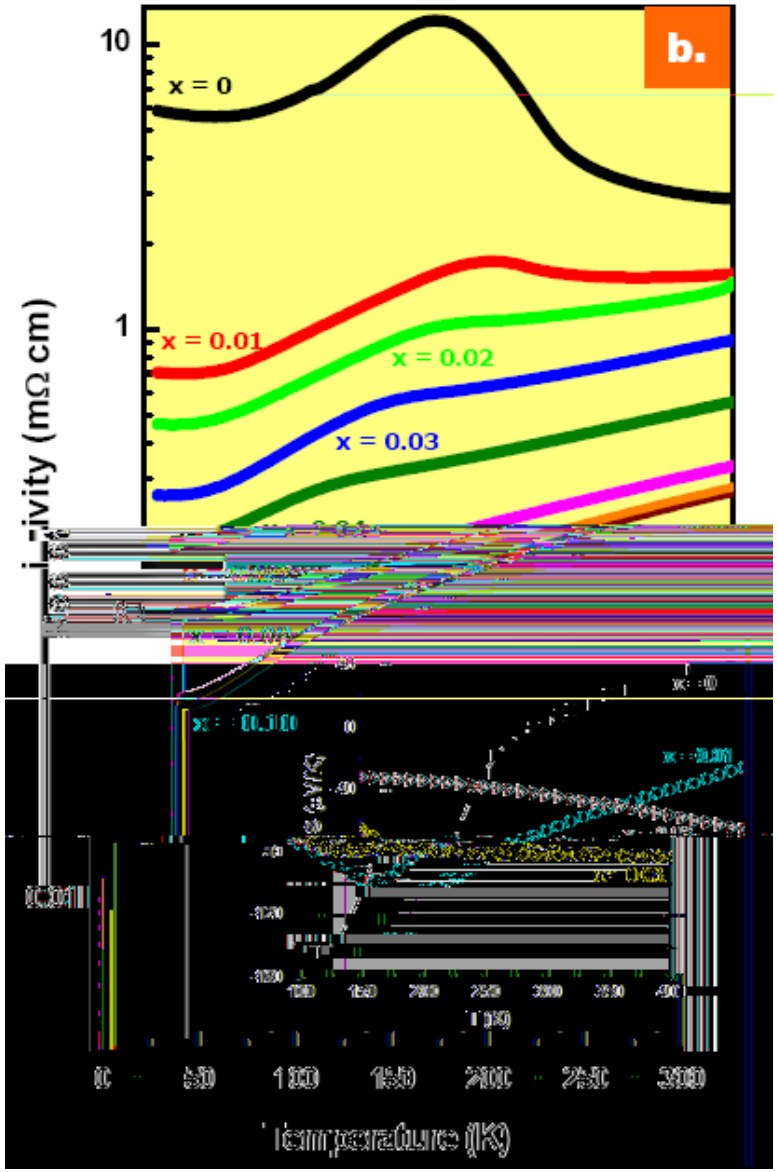
0.8
0.6
0.4
0.2
0
5000
10000
15000
20000

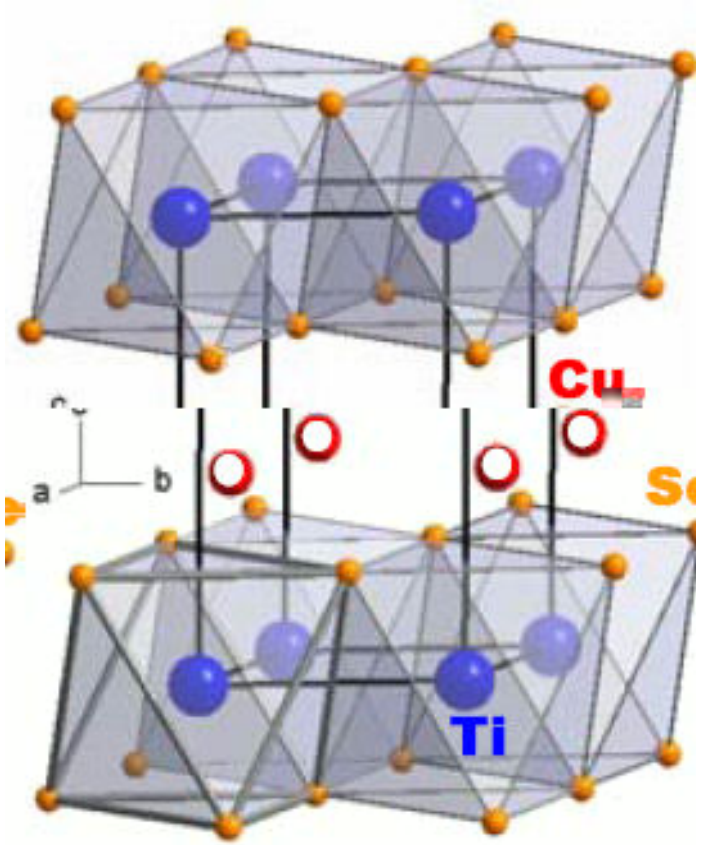
Newly discovered Cu_xTiSe_2





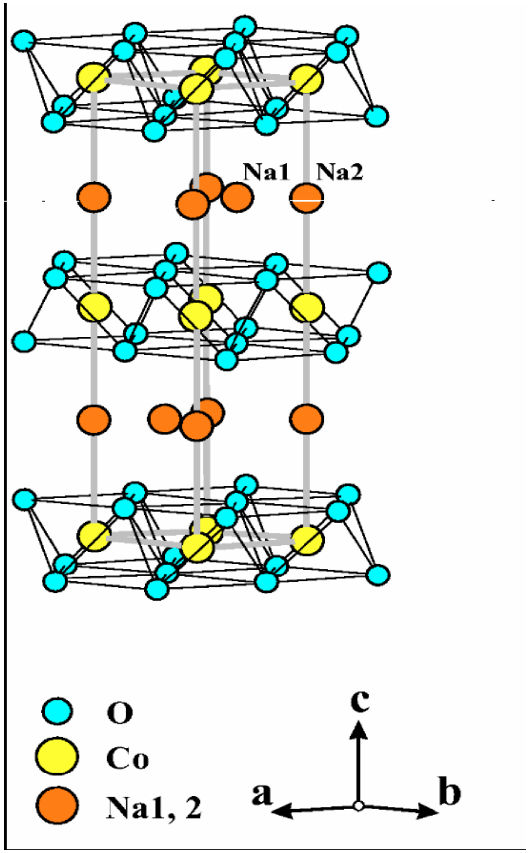
Cava group, Nature Phys. 06

Only superconductor
with 1T structure



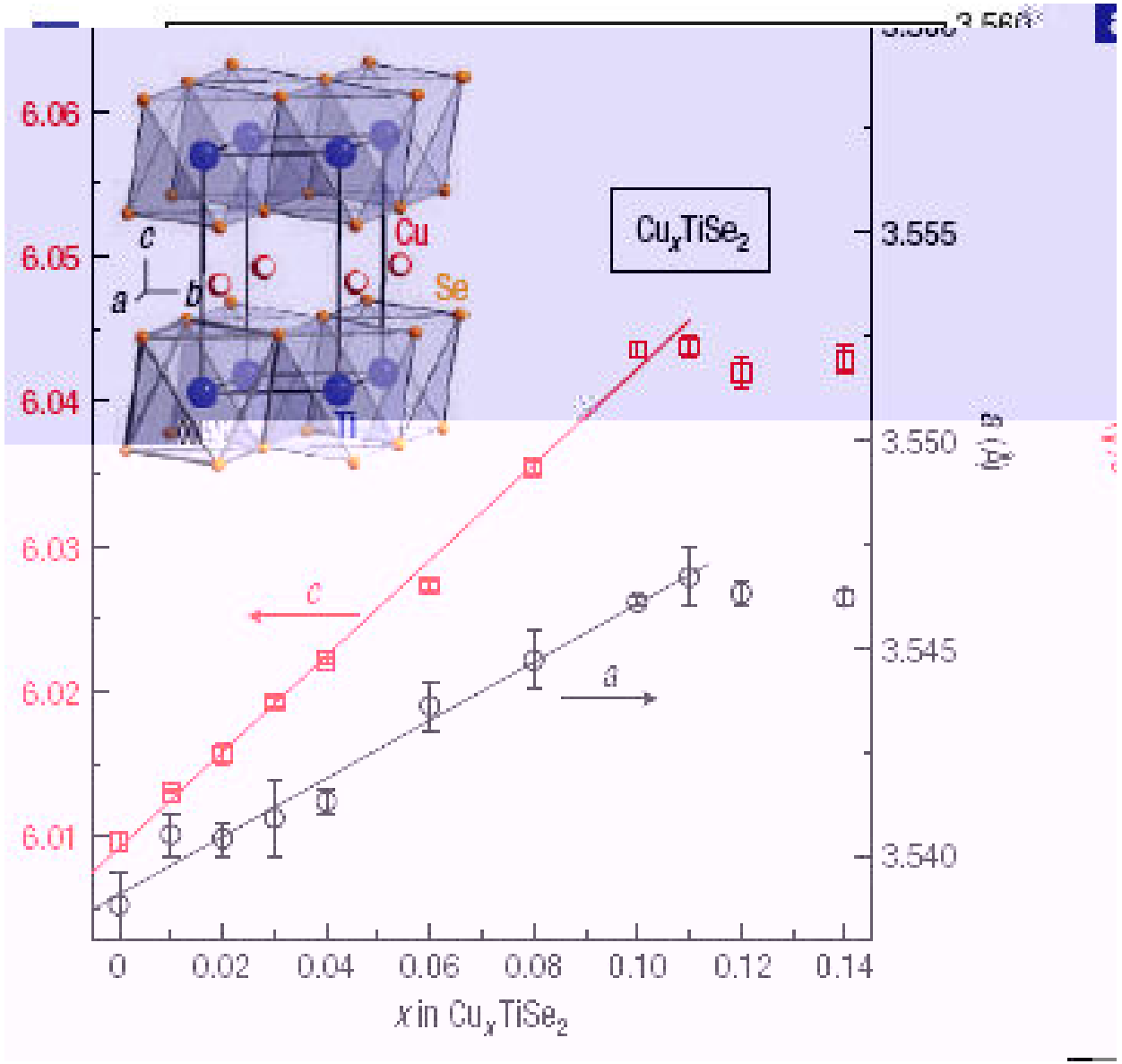
Na_xCoO_2

a=2.84 A c=10.81 A,
space group: P6/mmc



2H + 1T structural block

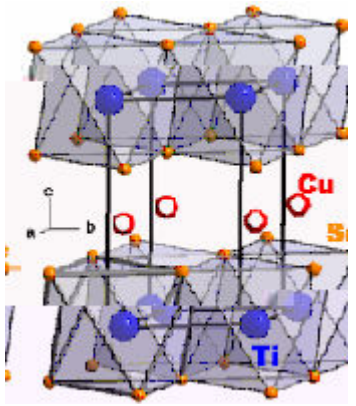
Lattice parameter with x, space group $P3m1$

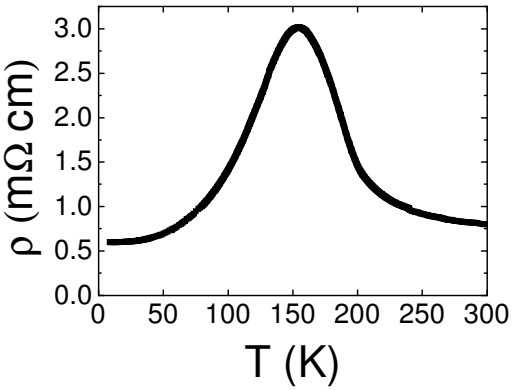


Parent compound 1T-TiSe2

- 1T-TiSe2 was one of the first CDW-bearing materials

- Broken symmetry at 200 K with a 2x2x2 superlattice





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Band structure and lattice instability of $TiSe_2$

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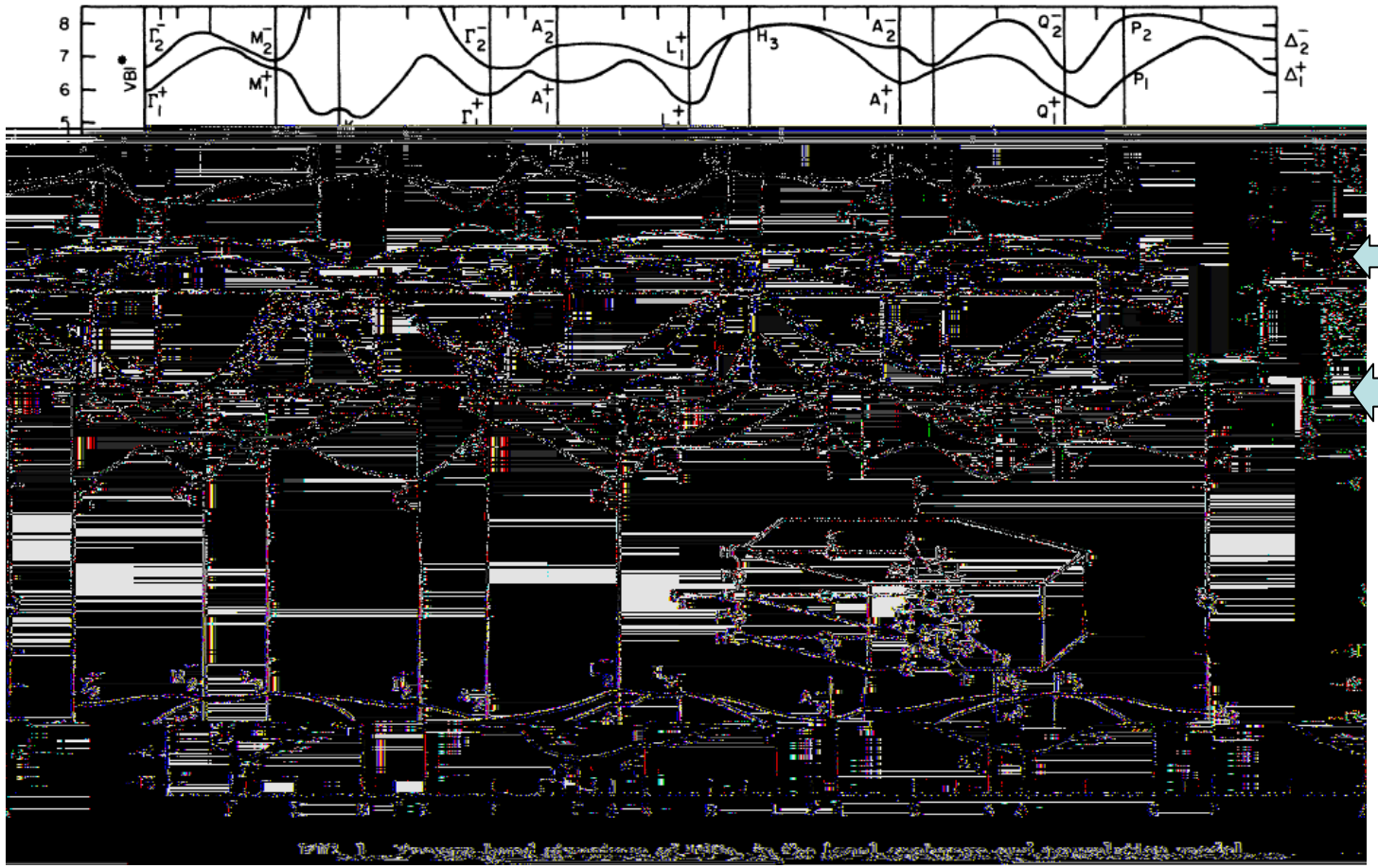
Materials Research Center, Northwestern University, Evanston, Illinois 60201 and Department of Physics and Astronomy and Argonne National Laboratory, Argonne, Illinois 60439

(Received 30 June 1977)



Ti: $3d^2 4s^2$

Se: $4s^2 4p^4$

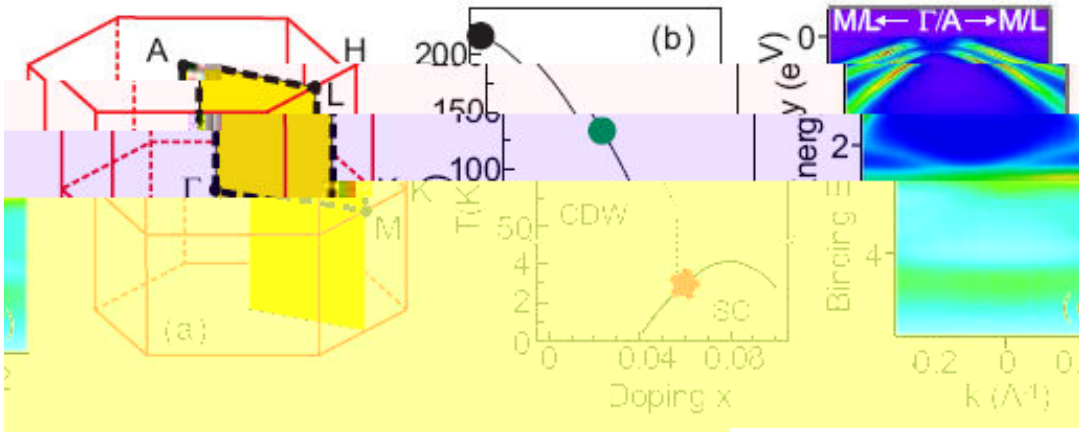
Ti : 3d band

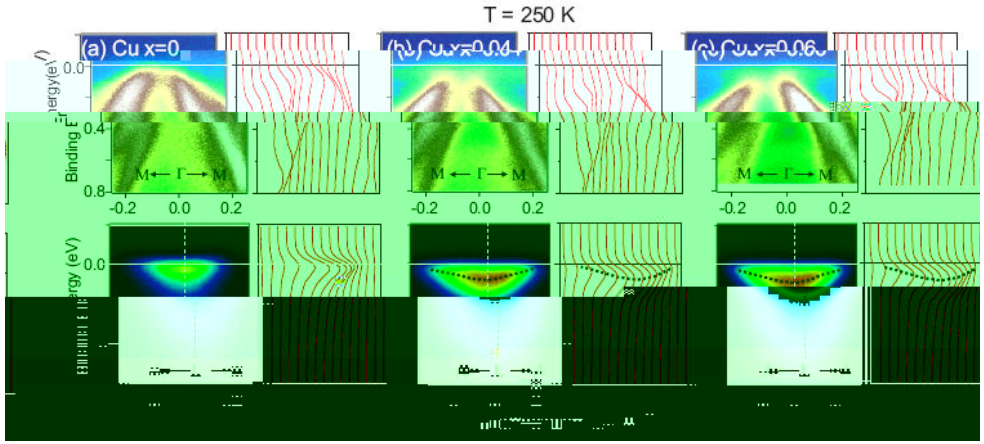
Se: 4p band

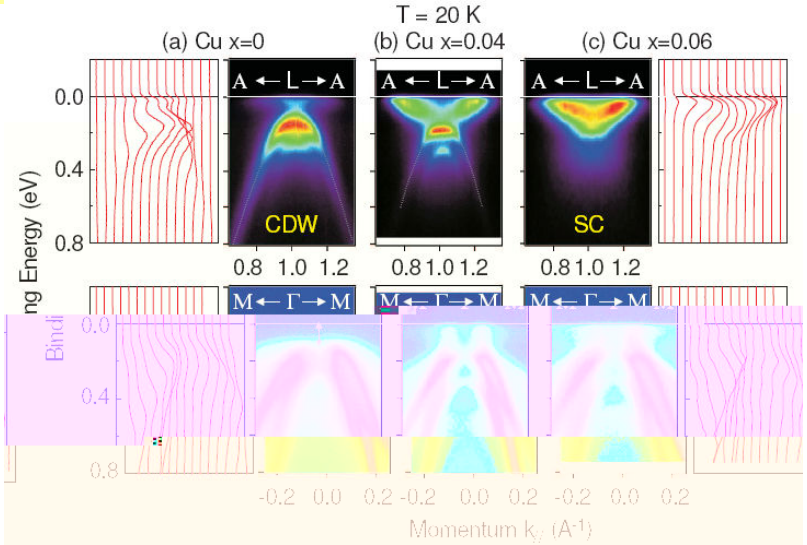
Emergence of Fermi Pockets in a New Excitonic Charge-Density-Wave Melted Superconductor

D. Qian,[1] D. Hsieh,[1] L. Wray,[1] E. Morosan,[2] N. L. Wang,[3] Y. Xia,[1] R. J. Cava,[2] and M. Z. Hasan[1,4,*]

[1]Department of Physics, Joseph Henry Laboratories of Physics, Princeton University, Princeton, New Jersey 08544, USA
[2]Department of Chemistry, Princeton University, Princeton, New Jersey 08544, USA
[3]Institute of Physics, Chinese Academy of Sciences, Beijing 100080, China







Electron-Hole Coupling and the Charge Density Wave Transition in $TiSe_2$

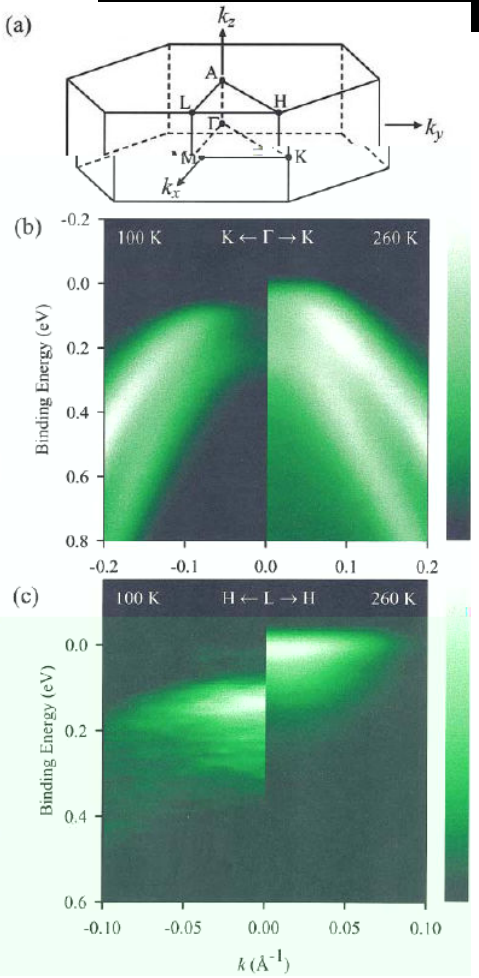
T. E. Kidd,[1] T. Miller,[1] M. Y. Chou,[2] and T.-C. Chiang[1,*]

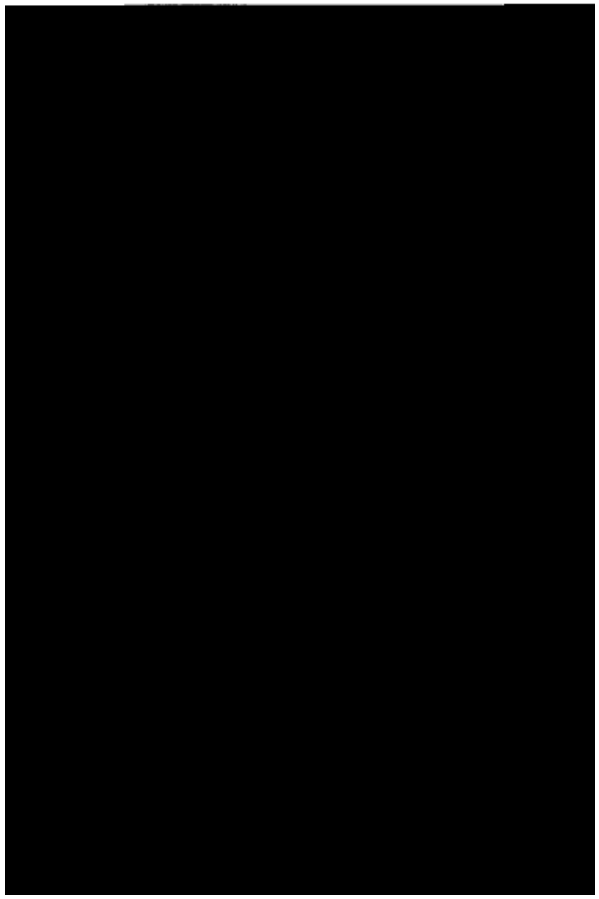
[1]Department of Physics, University of Illinois at Urbana-Champaign, 1110 West Green Street, Urbana, Illinois 61801-3080

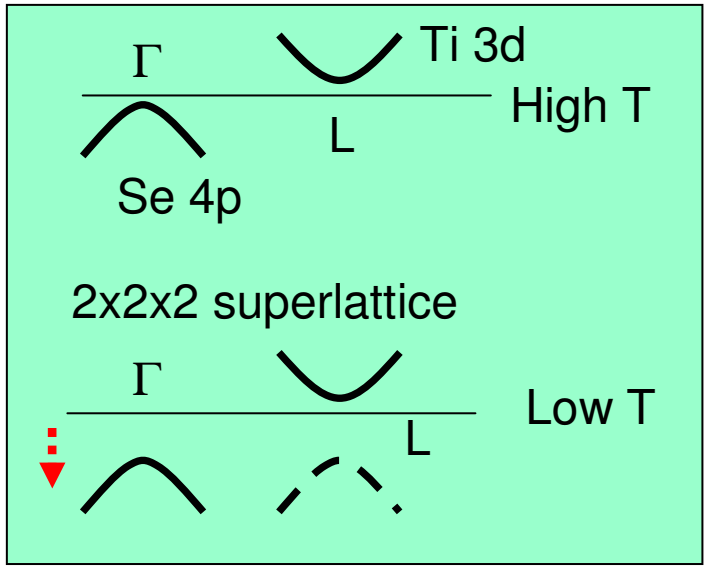
104 South Goodwin Avenue, Urbana, Illinois 61801-2902

[2]School of Physics, Georgia Institute of Technology, Atlanta, Georgia 30

(Received 8 November 2001; published 17 May 2002)





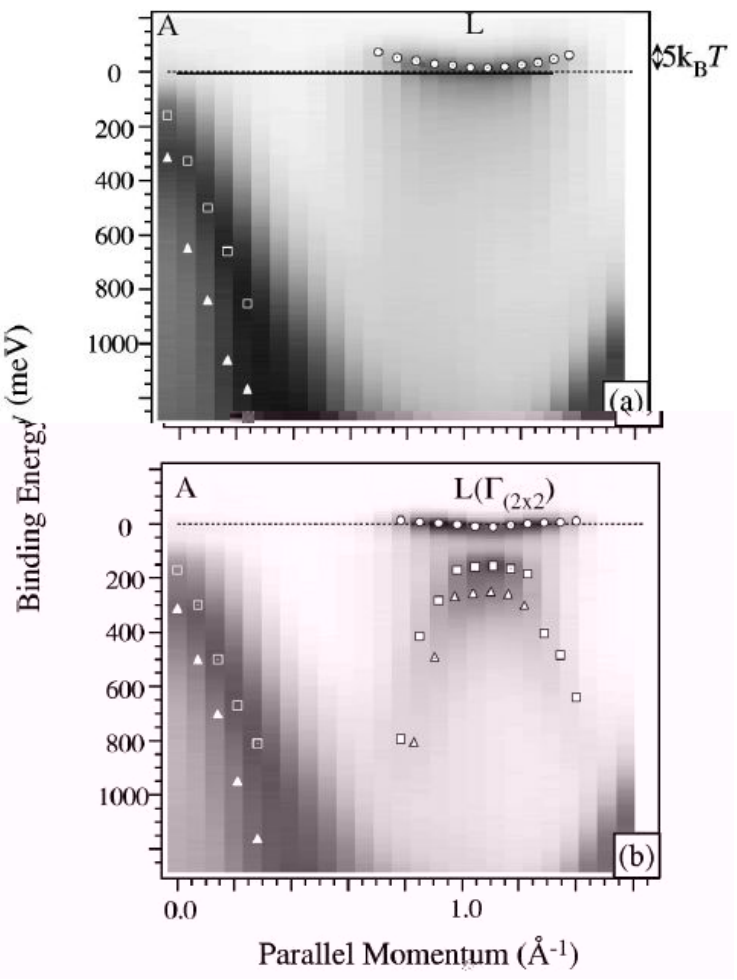


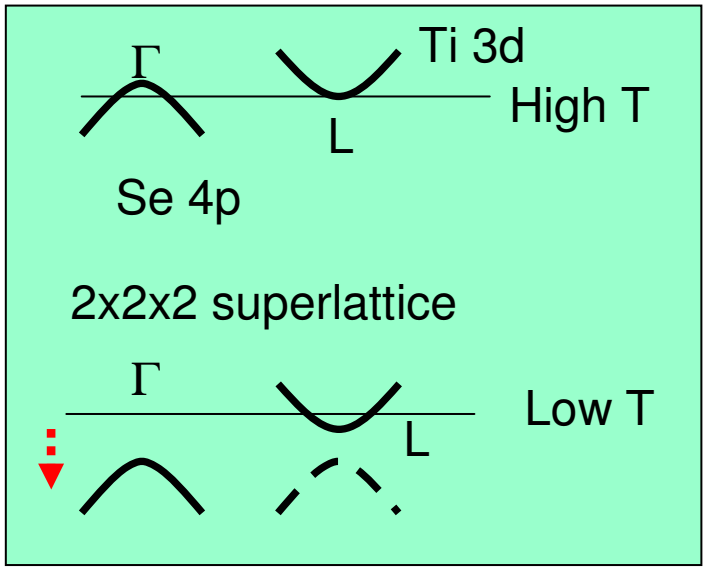
No band crossing
Fermi level below CDW.

It is insulating!!

Photoemission of bands above the Fermi level: The unoccupied electronic structure of 1T-TiSe$_2$

Th. Pillo, et al. PRB (2000)





metallic picture

But does not satisfy the charge neutrality!!

X

Issue

- ARPES experiments did not resolve conclusively whether the compound is a semimetal or semiconductor with a small indirect gap.

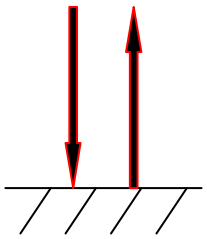
- The mechanism of the CDW transition:

  not due to the Fermi Surface nesting or saddle-point singularity

Optical measurement

Experiment

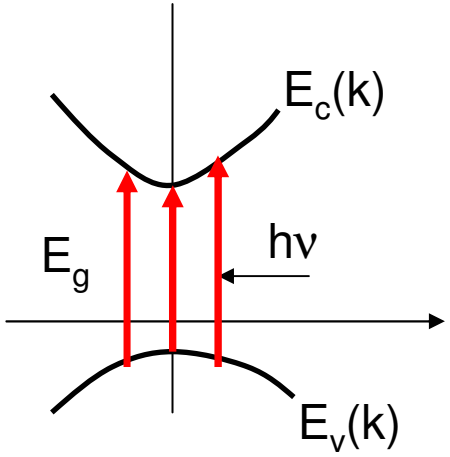
Reflectivity R(ω)



Interband transition

$|v,k>, E_v(k)$

$|c,k>, E_c(k)$



$$\hbar\omega = E_c(k) - E_v(k) \equiv E_{cv}(k)$$

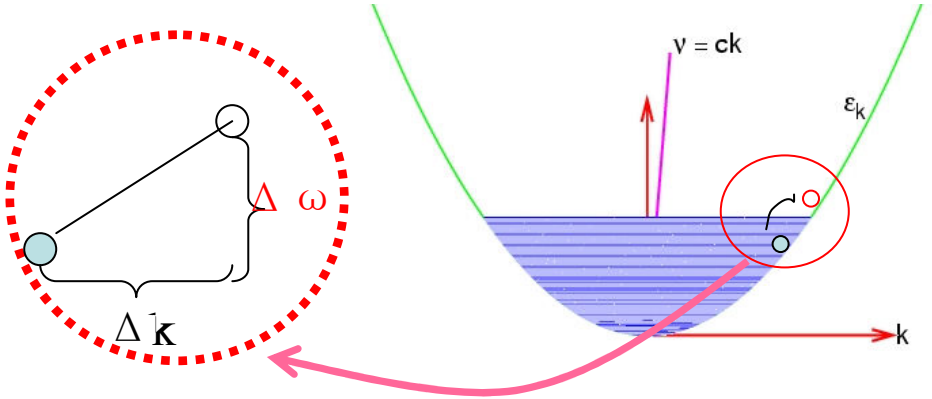
$$J(E) = \frac{V}{(2\pi)^3}\int \frac{ds}{|\nabla_k E_{cv}(k)|}$$

Kubo-Greenwood formula

$$\varepsilon_2(\omega) = \frac{8\pi^2 e^2}{m^2\omega^2} J(\hbar\omega)\,|\,\vec{p}_{vc}(\hbar\omega)\,|^2$$

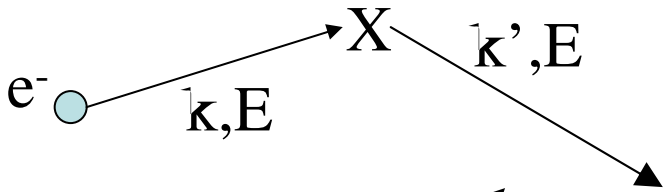
$$\sigma_1(\omega) = \frac{1}{4\pi}\omega\varepsilon_2(\omega)$$

Intraband transition

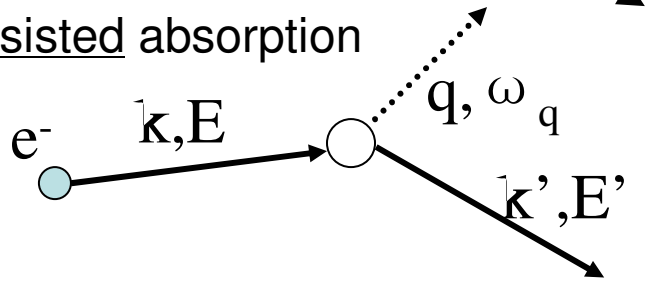


Infrared light cannot be absorbed directly by electron-hole excitation.

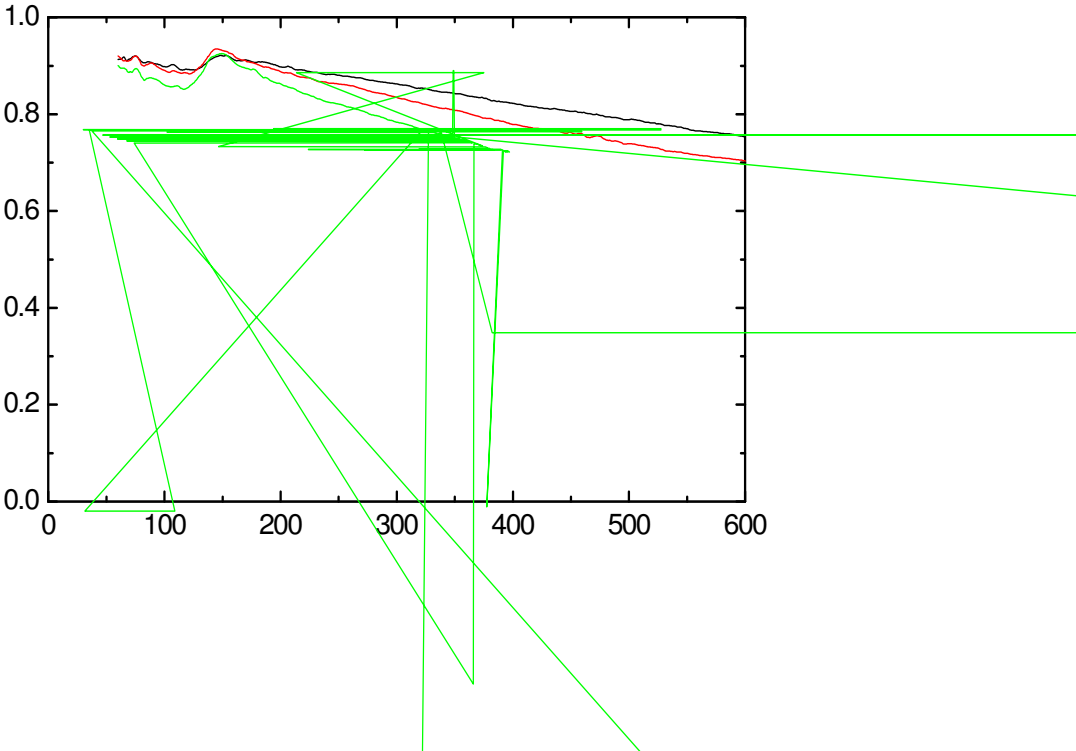
(a) Impurity-assisted absorption



(b) boson-assisted absorption



Holstein process, if phonons are involved.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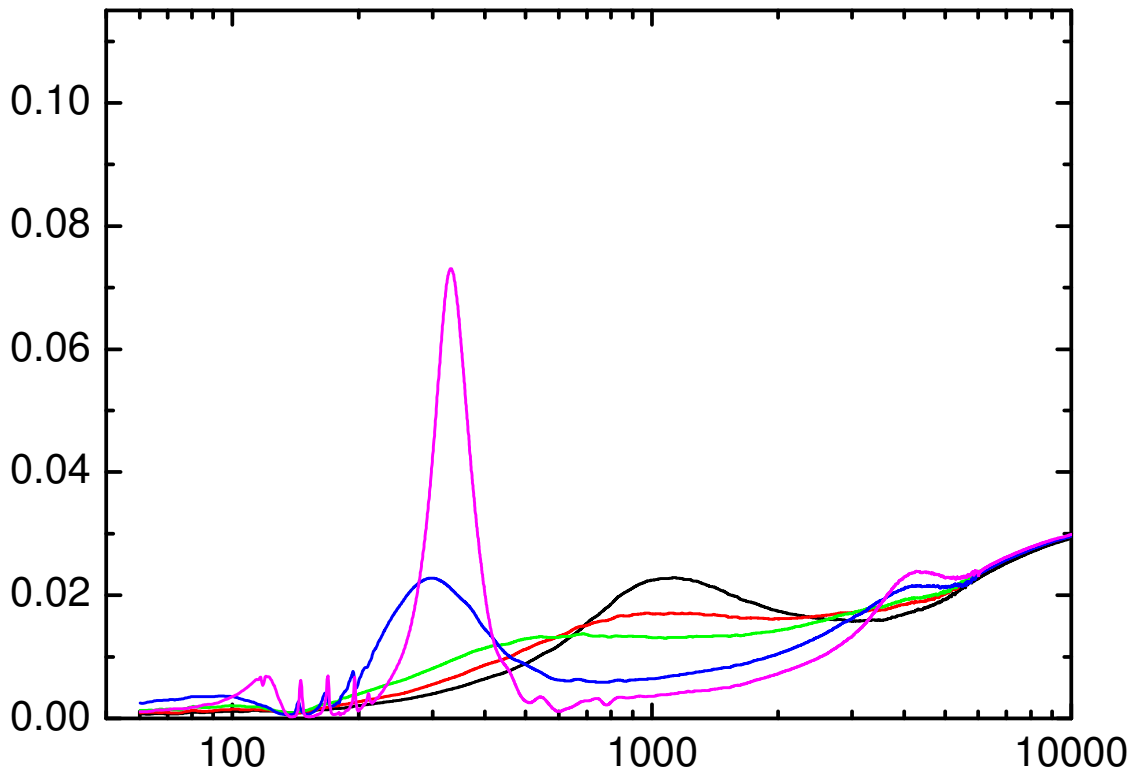
0.4
0.2
0.0
0
100
200
300
400
500
600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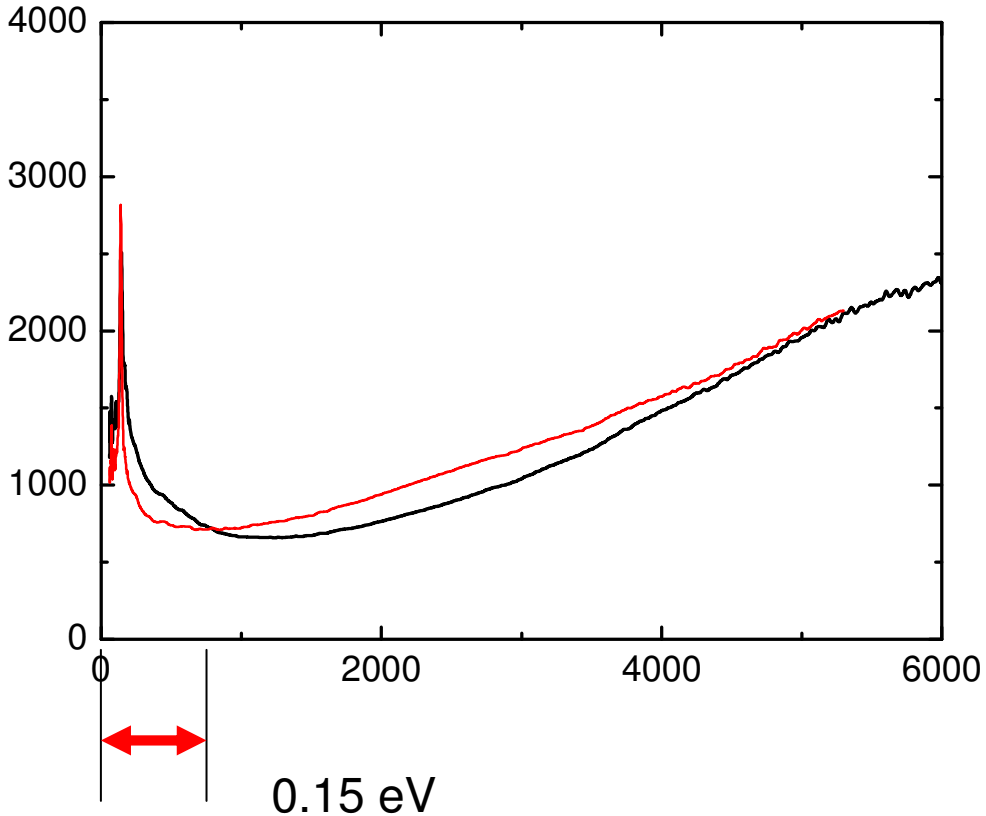
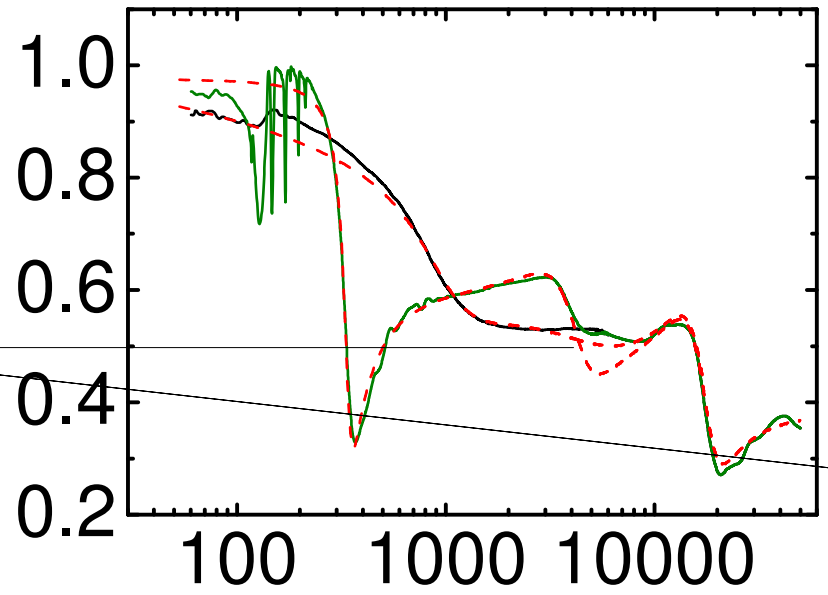
0.08
0.06
0.04
0.02
0.00
100
1000
10000



Free carriers with very long relaxation time exist in the CDW gapped state

⇨ FS is not fully gapped??


1.0
0.8
0.6
0.4
0.2
100
1000
10000

- **1T TiSe2 is a semimetal with very low carrier density at all T**

- **Carrier density changes with T decreases from room T to ☛ 0 K then increases slightly with further decreasing T**

- **Development of an energy gap ~0.☛ eV below 200 K**

- **Dramatic different carrier damping at different T**

Excitonic Phases W. Kohn, PRL 67

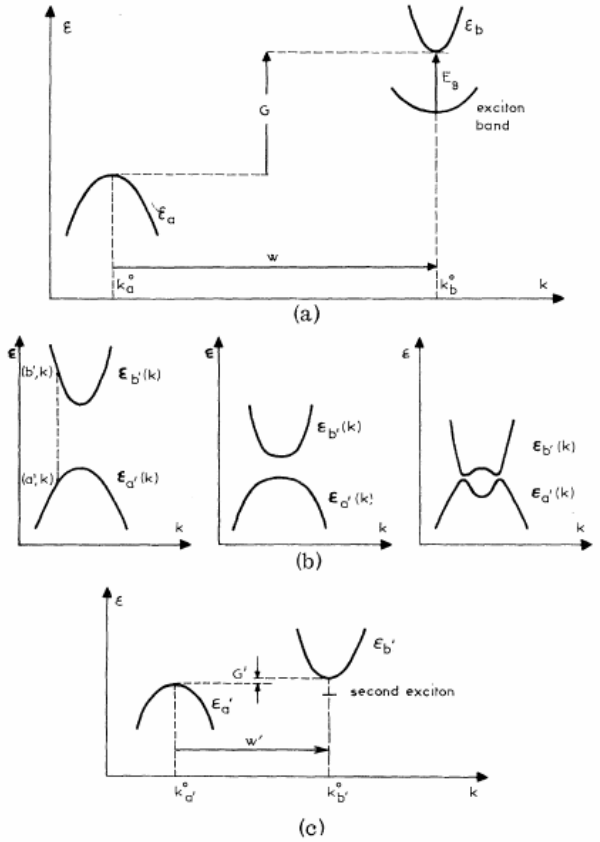


FIG. 1. The insulating side. (a) Energy bands and exciton band of the normal insulator. (b) The new energy bands after the first excitonic transition for successive values of the external parameter (e.g., pressure). (c) The second excitonic instability.

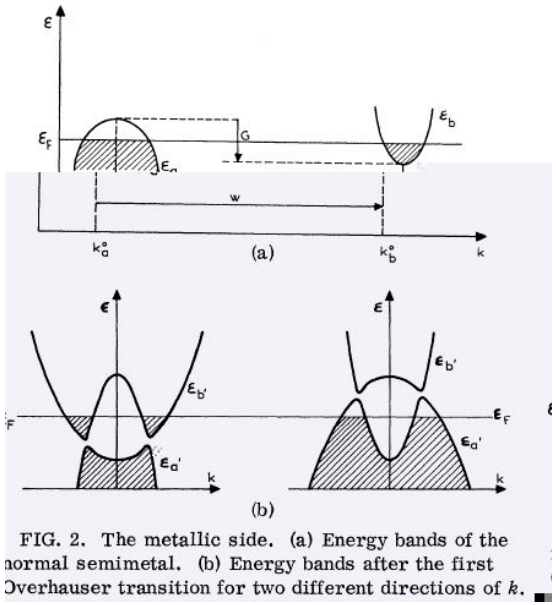


FIG. 2. The metallic side. (a) Energy bands of the normal semimetal. (b) Energy bands after the first Overhauser transition for two different directions of k.

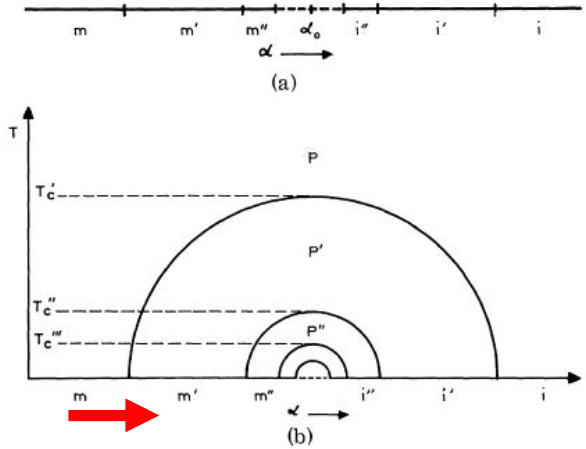


FIG. 3. The excitonic phases. (a) Succession of phases, at $T=0°$, for different values of α; m, metallic; i, insulating. The dotted interval contains an infinity of m and i phases. (b) Total phase diagram, showing an infinity of nested phases.

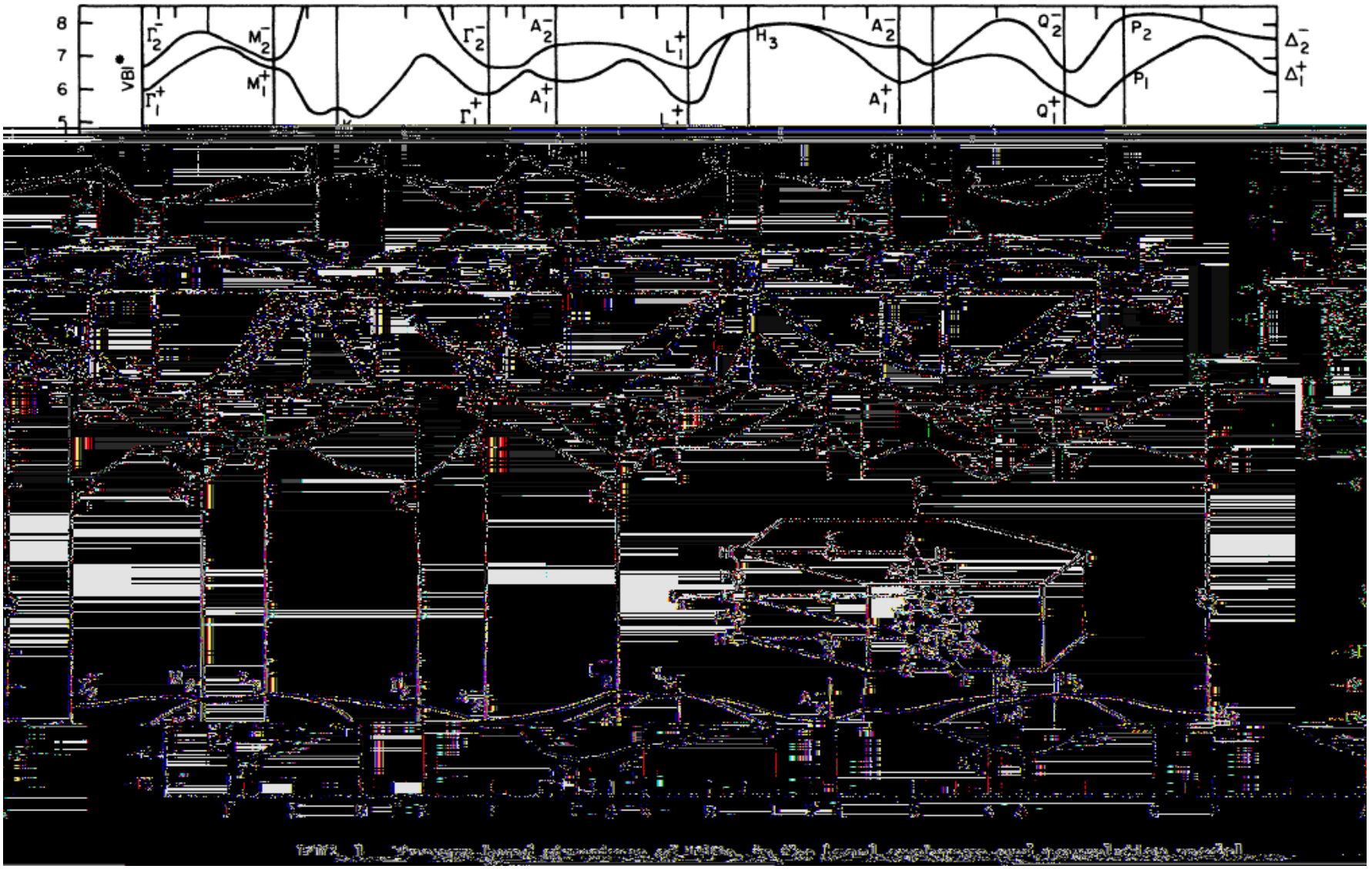
The electron-hole coupling acts to mix the electron ban

$$\frac{2}{p} \quad 4 \quad {}^{2}\left(\frac{h}{h} \quad \frac{e}{e}\right)$$

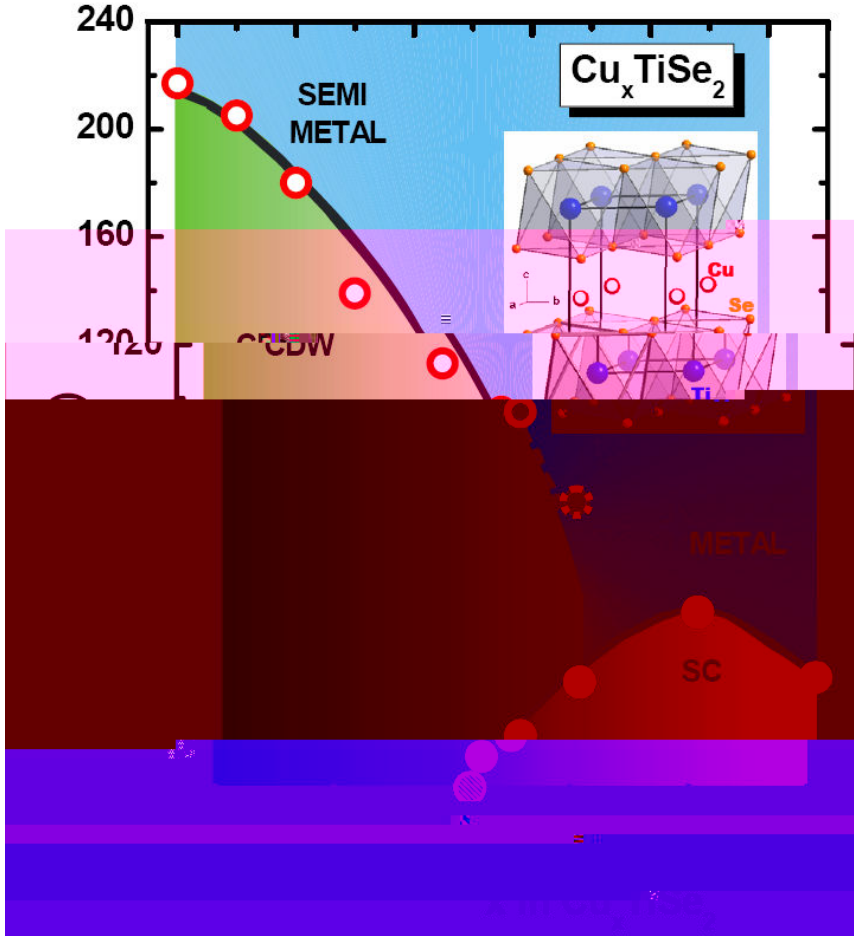
$$R_H = \frac{1}{e}\frac{n_h\mu_h^2 - n_e\mu_e^2}{(n_h\mu_h + n_e\mu_e)^2},$$

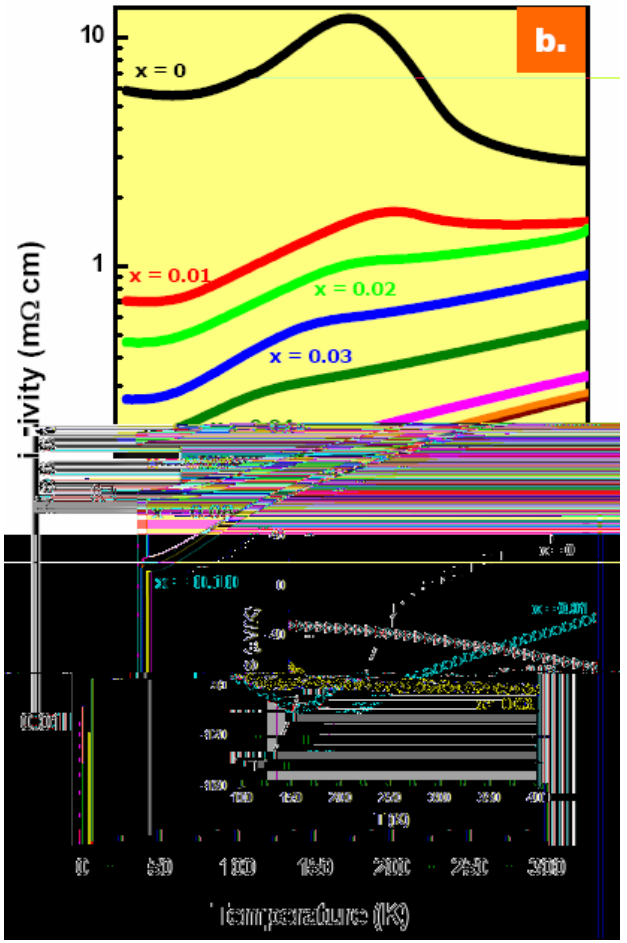
$$\sigma = e(n_h\mu_h + n_e\mu_e)$$

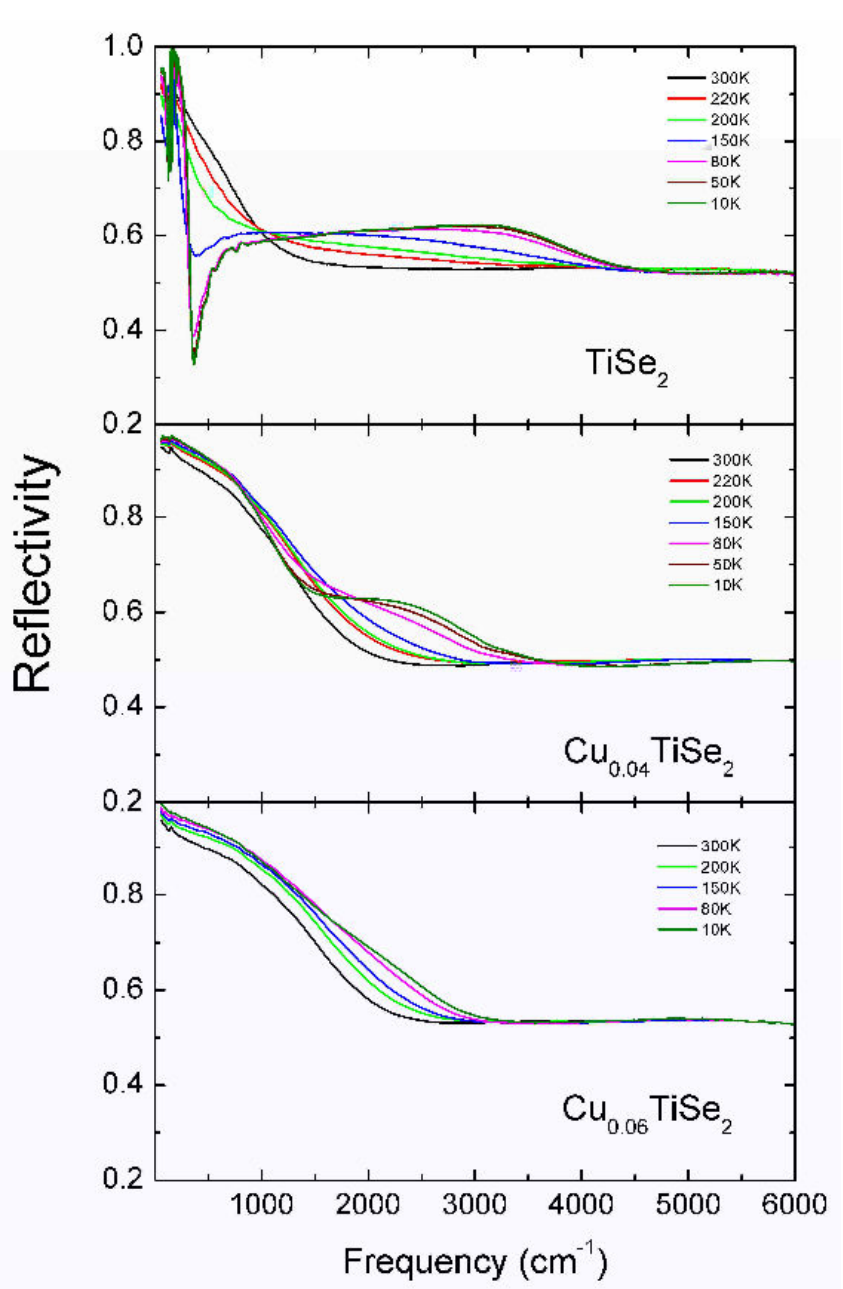
Exciton-driven CDW

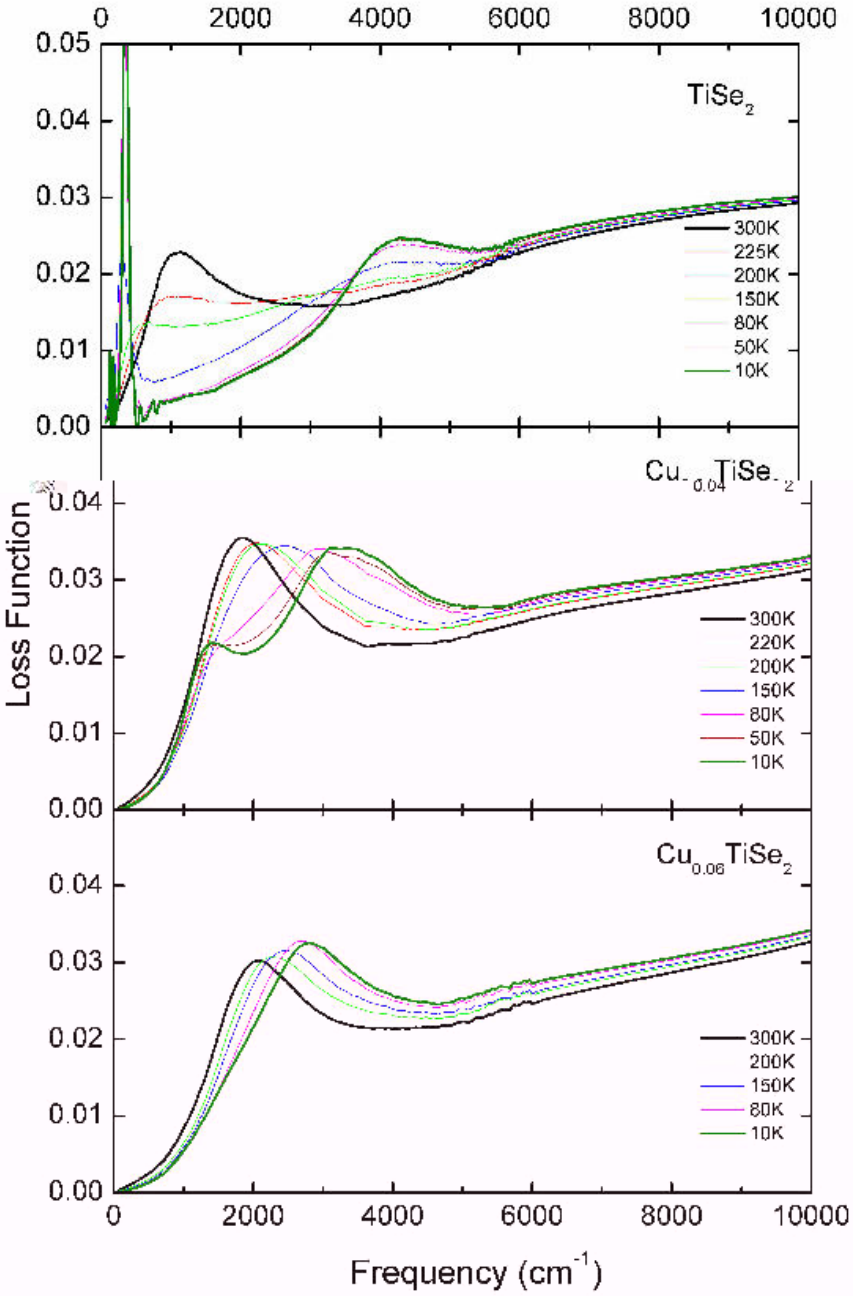

8
7
6
VBM
Γ_2^-
Γ_1^+
M_2^-
M_1^+
K
Γ_2^-
Γ_1^+
A_2^-
A_1^+
L_1^+
L_1^+
H_3
A_2^-
A_1^+
Q_2^-
Q_1^+
P_2
P_1
Δ_2^-
Δ_1^+

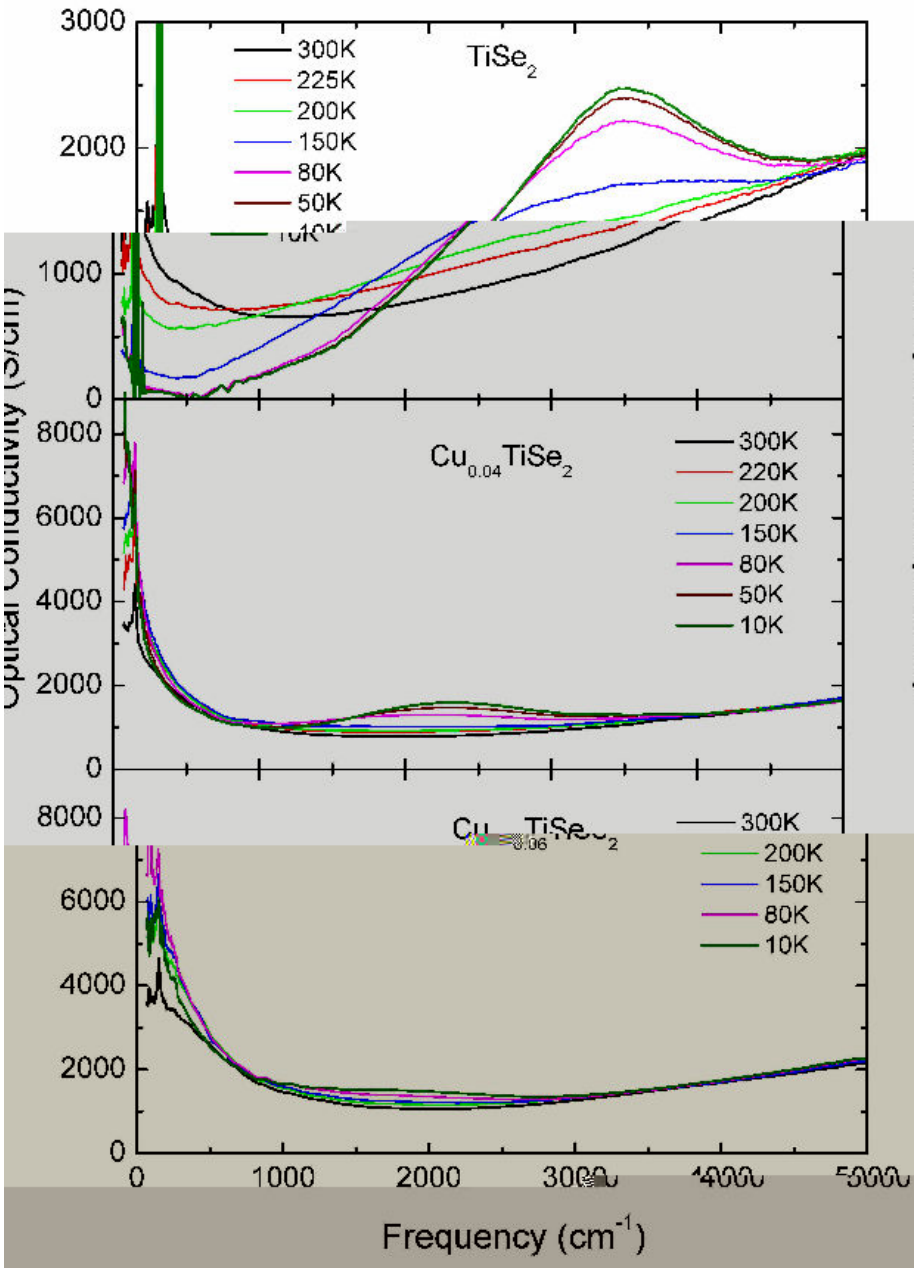
Cu-doped CuxTiSe2

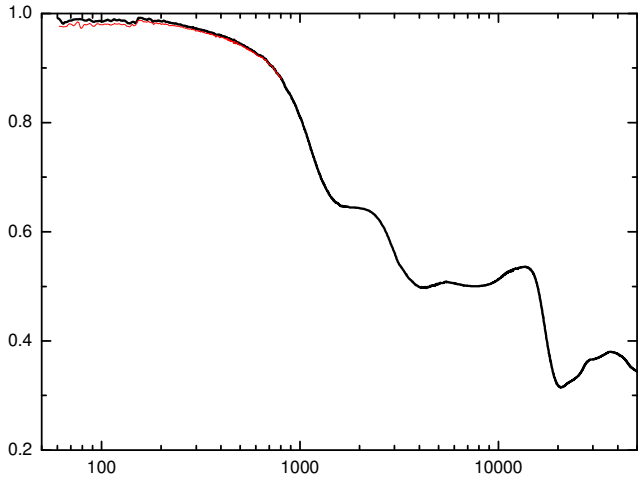


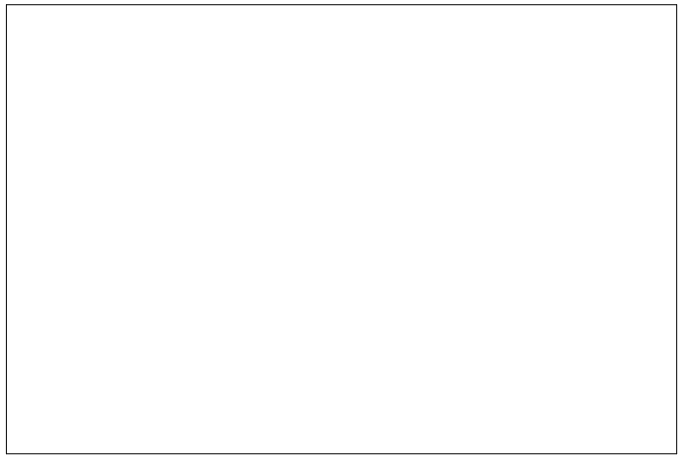


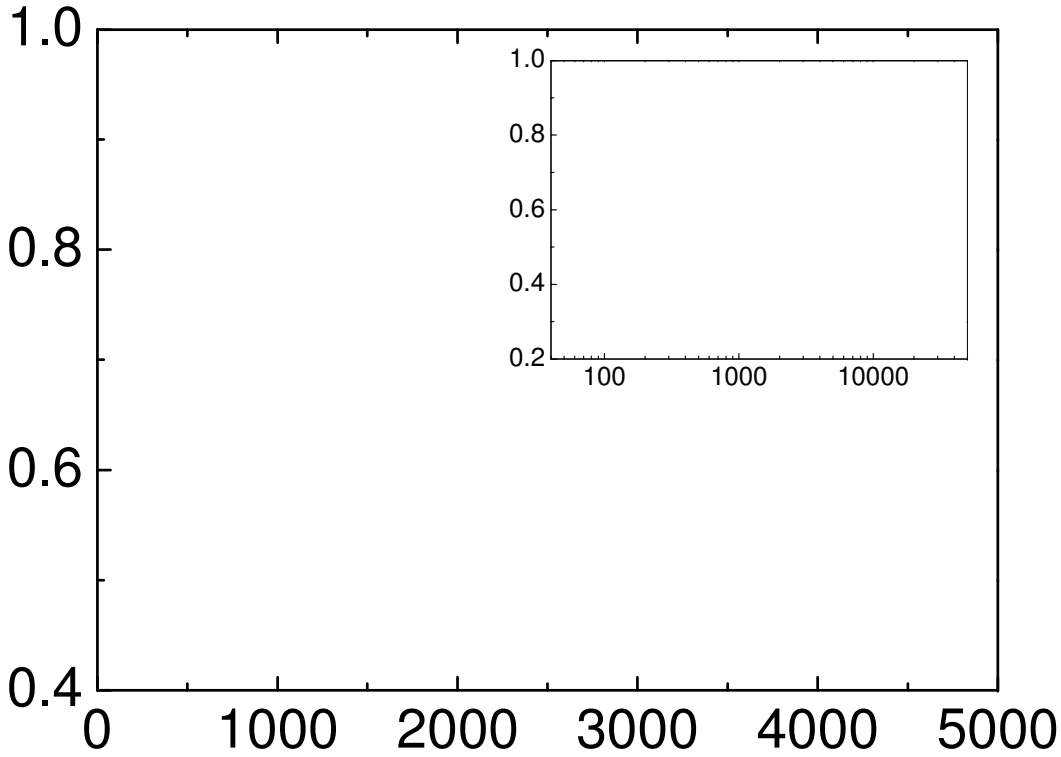

Reflectivity
TiSe2
Cu0.04TiSe2
Cu0.06TiSe2
300K
220K
200K
150K
80K
50K
10K
Frequency (cm-1)

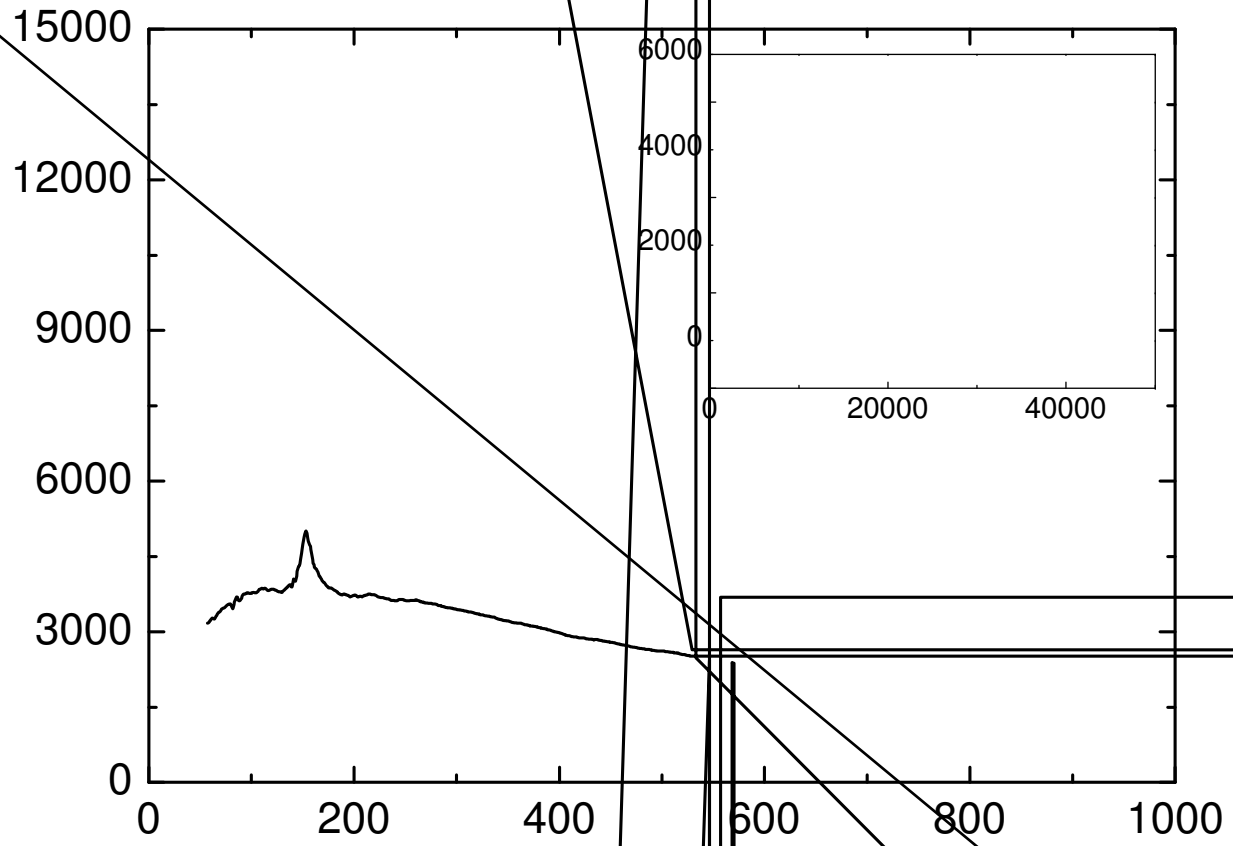

Loss Function
TiSe2
Cu0.04TiSe2
Cu0.06TiSe2
300K
225K
220K
200K
150K
80K
50K
10K
Frequency (cm-1)


TiSe2
300K
225K
200K
150K
80K
50K
Cu0.04TiSe2
300K
220K
200K
150K
80K
50K
10K
Cu0.06TiSe2
300K
200K
150K
80K
10K
Optical Conductivity (S/cm)
Frequency (cm-1)


1.0
0.8
0.6
0.4
0.2
100
1000
10000




1.0
0.8
0.6
0.4
0
1000
2000
3000
4000
5000
1.0
0.8
0.6
0.4
0.2
100
1000
10000


15000
12000
9000
6000
3000
0
0
200
400
600
800
1000
6000
4000
2000
0
0
20000
40000

Plasma frequency increases with decreasing T??

$$\omega_p^2 = \frac{4\pi n e^2}{m^*}$$

In terms of two bands:

$$\omega_p^2 = 4\pi e^2 \left(\frac{n_e}{m_e^*} + \frac{n_h}{m_h^*}\right)$$

- n increases with decreasing T??

- m* decreases with decreasing T, undressing effect??

Low-Temperature Anomalies and Ferromagnetism of EuB_6

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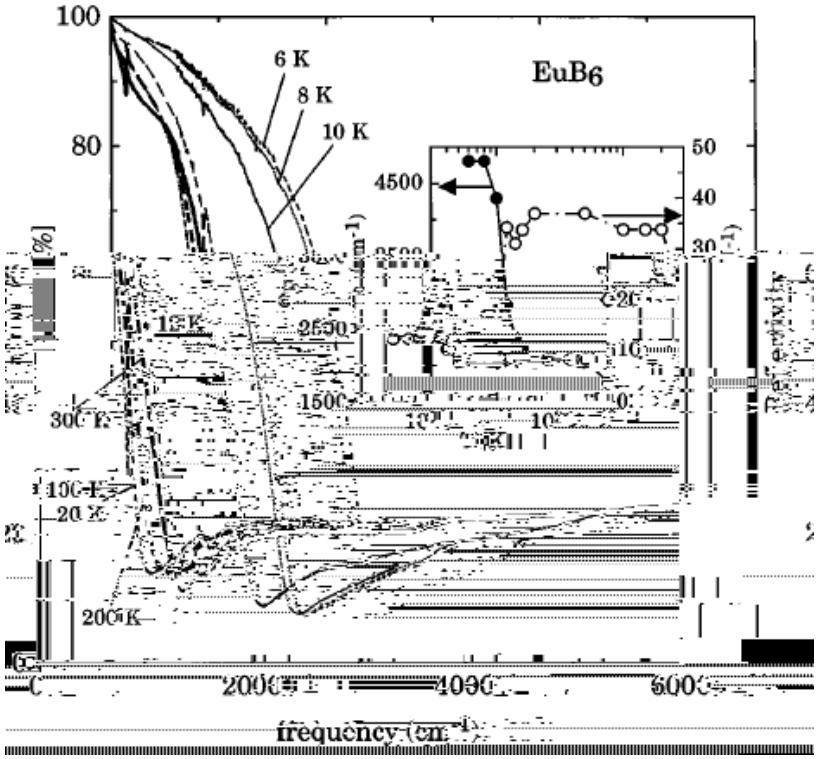
(Received 21 April 1997)



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Scaling between magnetization and Drude weight in EuB_6

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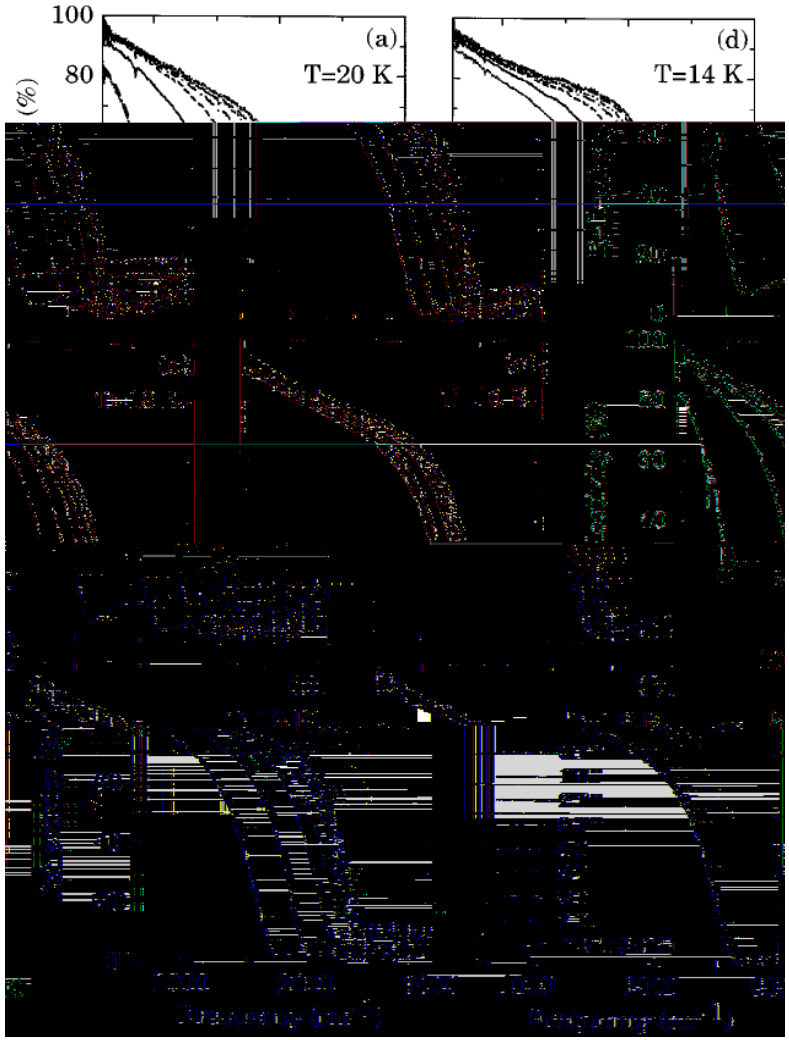
NHMFL, FSU, Tallahassee, Florida 32306



Ferromagnetism from Undressing

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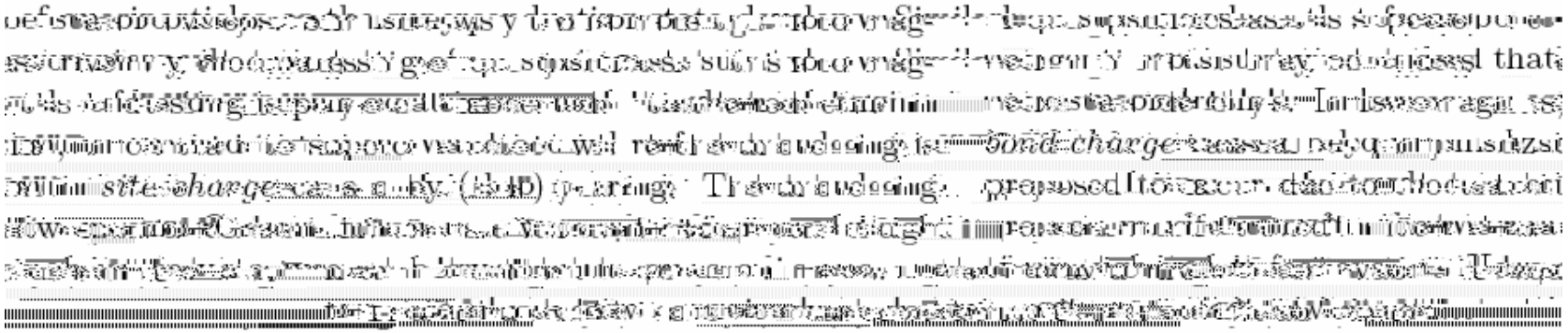
Department of Physics, University of California, San Diego
La Jolla, CA 92093-0319
(November 19, 2002)

We have recently proposed that superconductivity may be understood as driven by the undressing

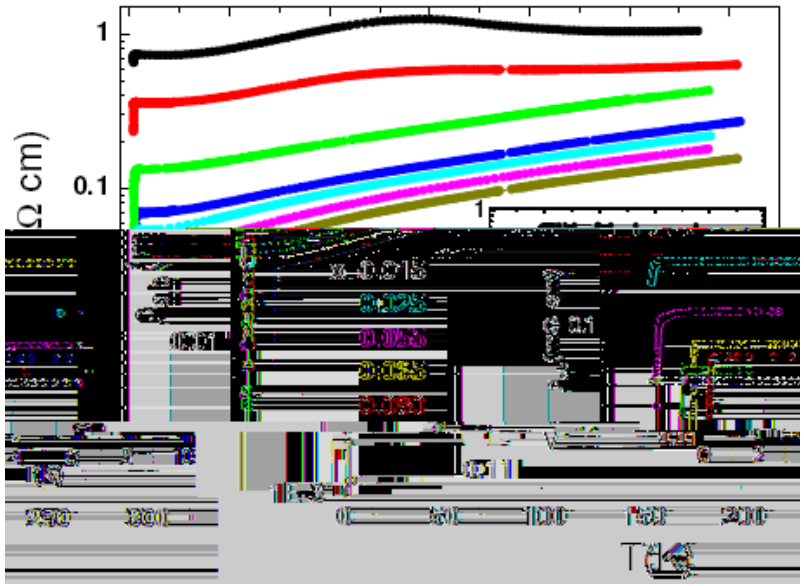


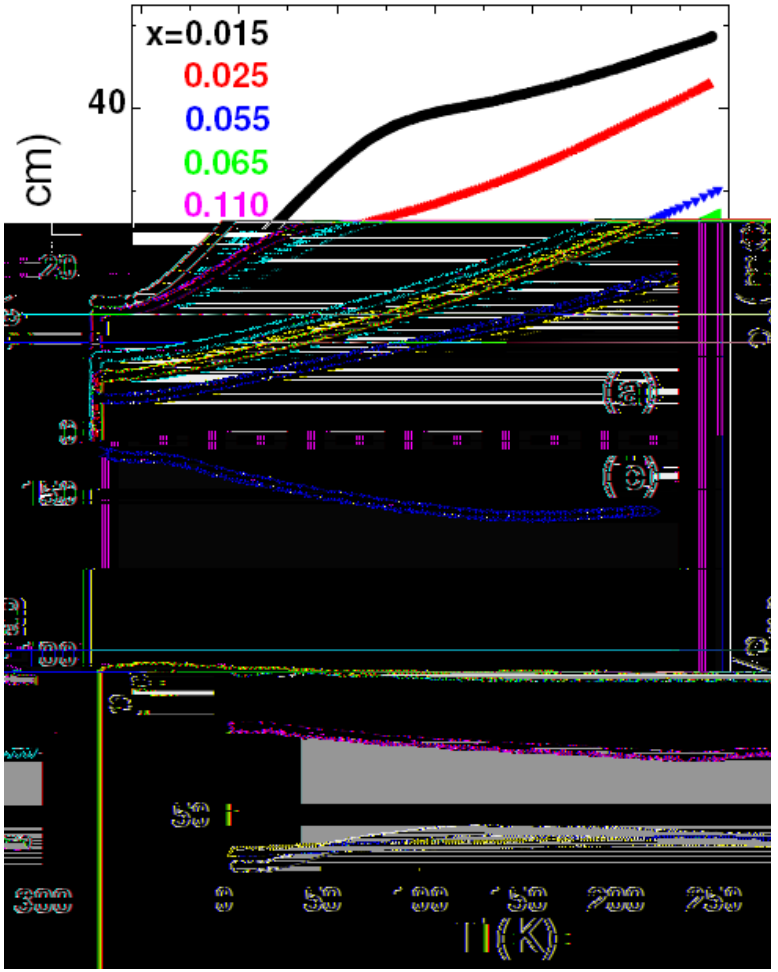
Cond-mat/0007454 (PRB (2000))

Transport properties in Cu_xTiSe_2 ($0.015 \leq x \leq 0.110$) Single Crystal

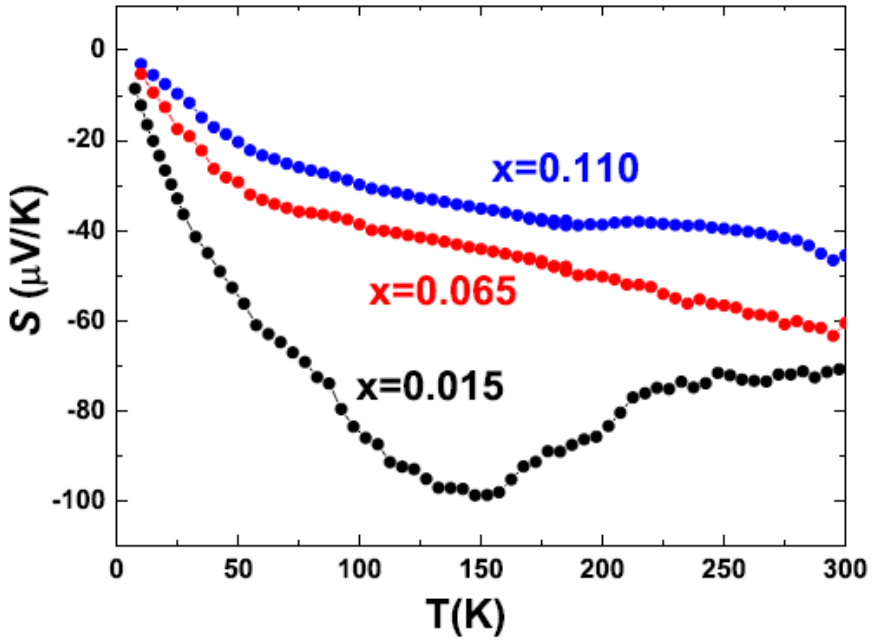
G. Wu, H. X. Yang, L. Zhao, X. G. Luo, T. Wu, G. Y. Wang and X. H. Chen*

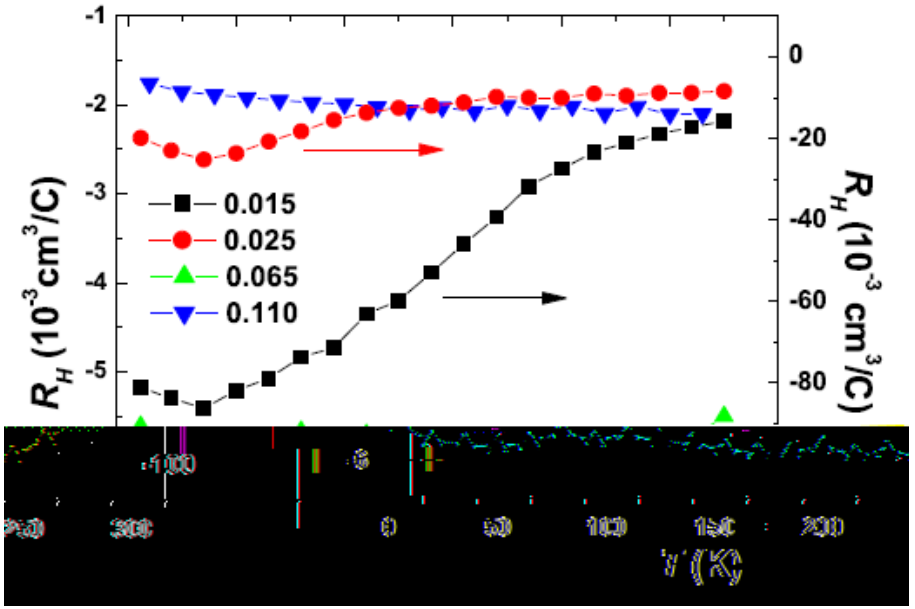
Hefei National Laboratory for Physical Science at Microscale and Department of Physics, University of Science and Technology of China, Hefei, Anhui 230026, People's Republic of China





Cond-mat/0703645





Hall coefficient is almost T-independent for superconducting sample!!