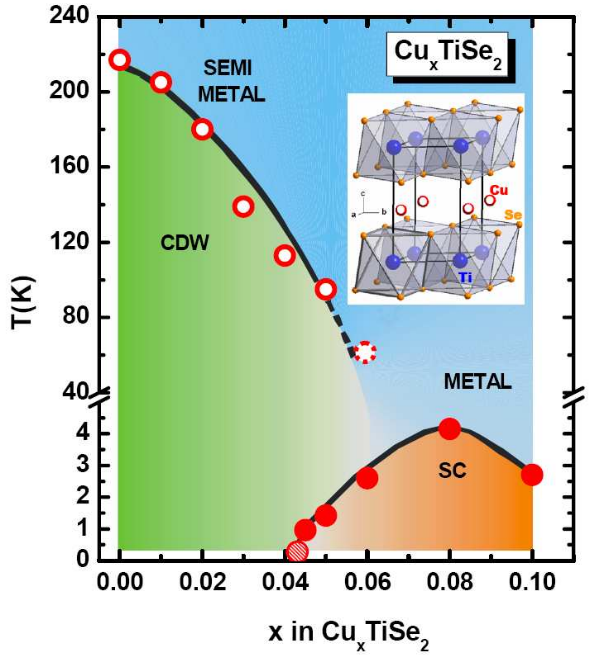
Optical study on CuxTiSe2

Nan Lin Wang

Institute of Physics, CAS



E. Morosan et al, Nature Phys. 06

Dedicated to 70th birthday of

Prof. ZhaoBin Su and Prof. Lu Yu

Outline

- Introduction to transition metal dichalcogenides
  - 1 T and 2 H phases
- **CDW mechanism of Parent compound 1T-$TiSe_2$**
  - excitonic
  - semimetal or semiconductor?
  - Kohn-Overhauser-type
- **Cu-doped compound Cu_xTiSe_2**
  - evolution
  - x=0.07, anomalous metallic state

Collaborators

G. Li, W. Z. Hu, J. Dong

Institute of Physics, CAS

E. Morosan, R. J. Cava

Department of Chemistry, Priceton University

CuxTiSe2 and other crystals

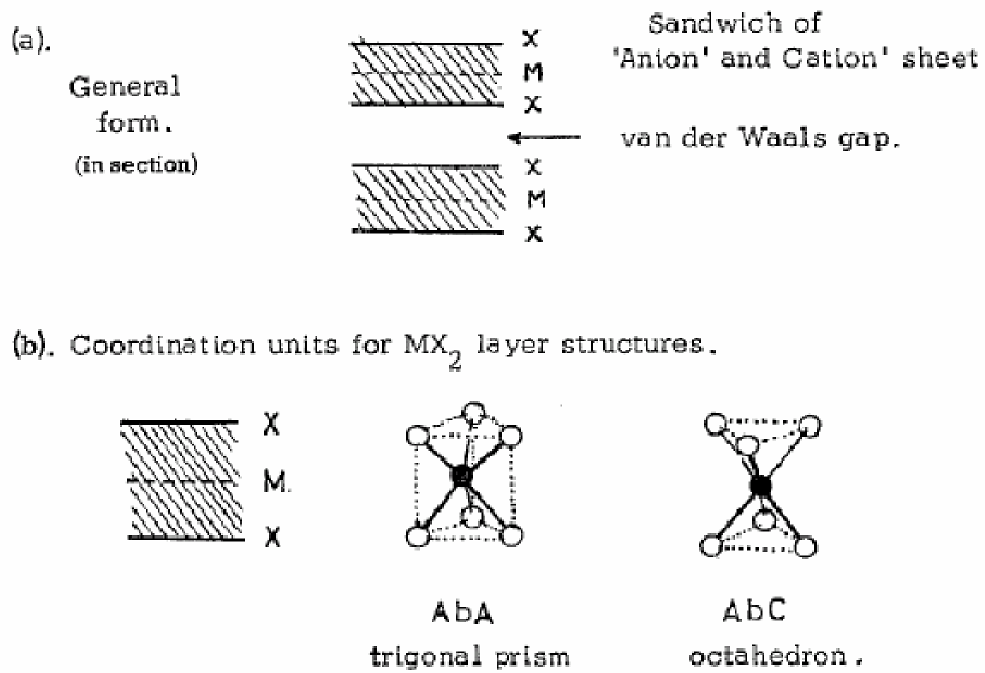
D. Qian, D. Hsieh, Z. Hasan

Department of Physics, Princeton University

ARPES

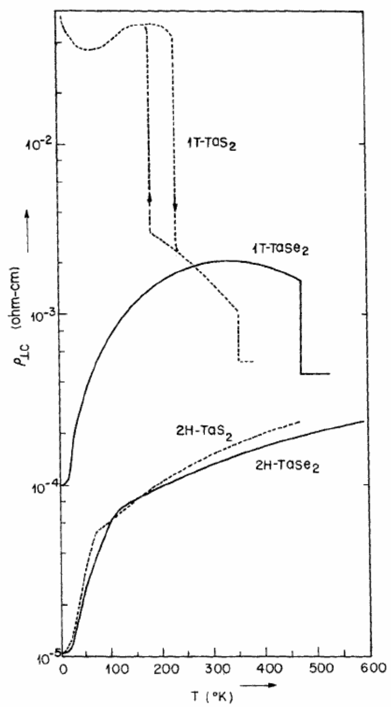
Helpful discussions with: W. Ku, Z. Q. Wang, T. M. Rice, L. Yin, T. Tohyama, R. S. Markiewicz, D. L. Feng, Q. H. Wang, X. C. Xie, and Lu Yu

structure

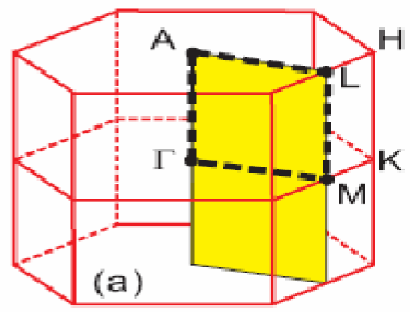


J. A. Wilson *et al.*

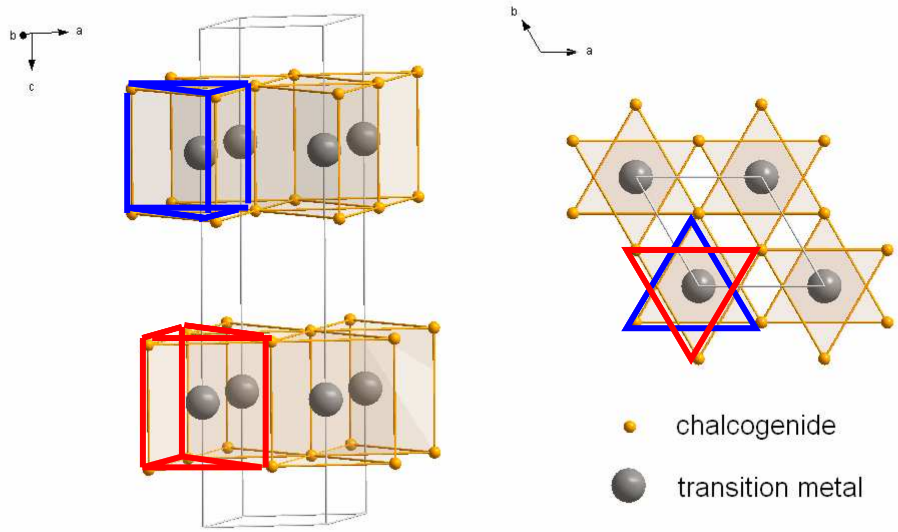
Fig. 3



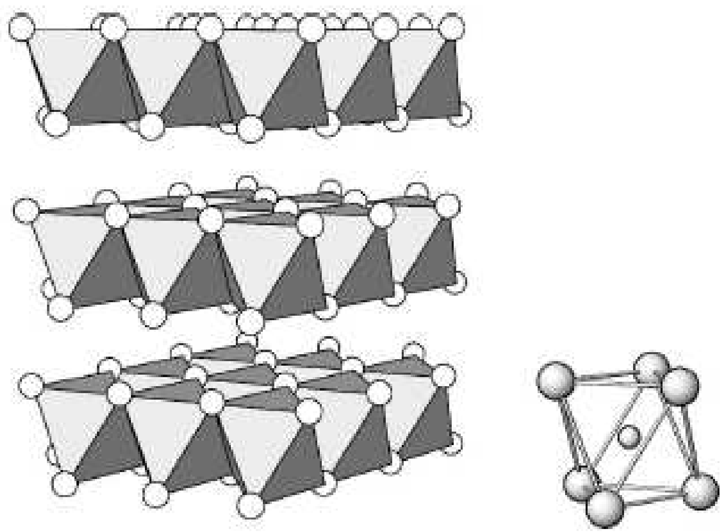
J.A.Wilson and A.D.Yoffe
Adv. Phys. 18, 193-335 (1969)



Brillouin zone

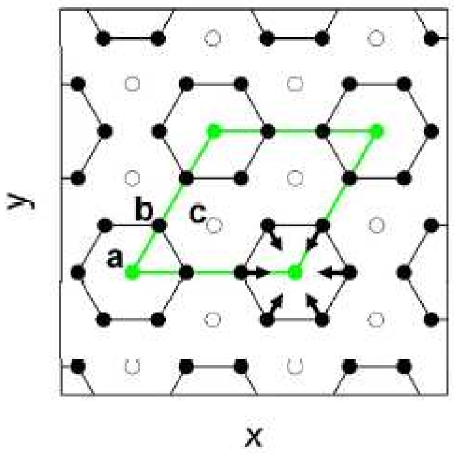


2***H*** type: ***H****exagonal*

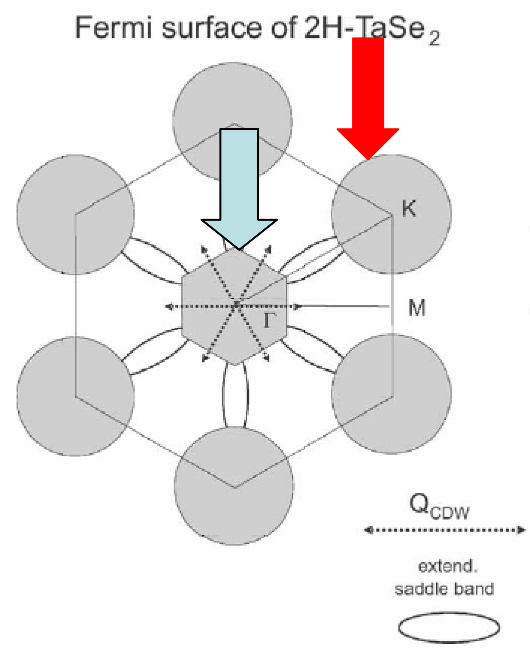


1*T* type: *Trigonal*

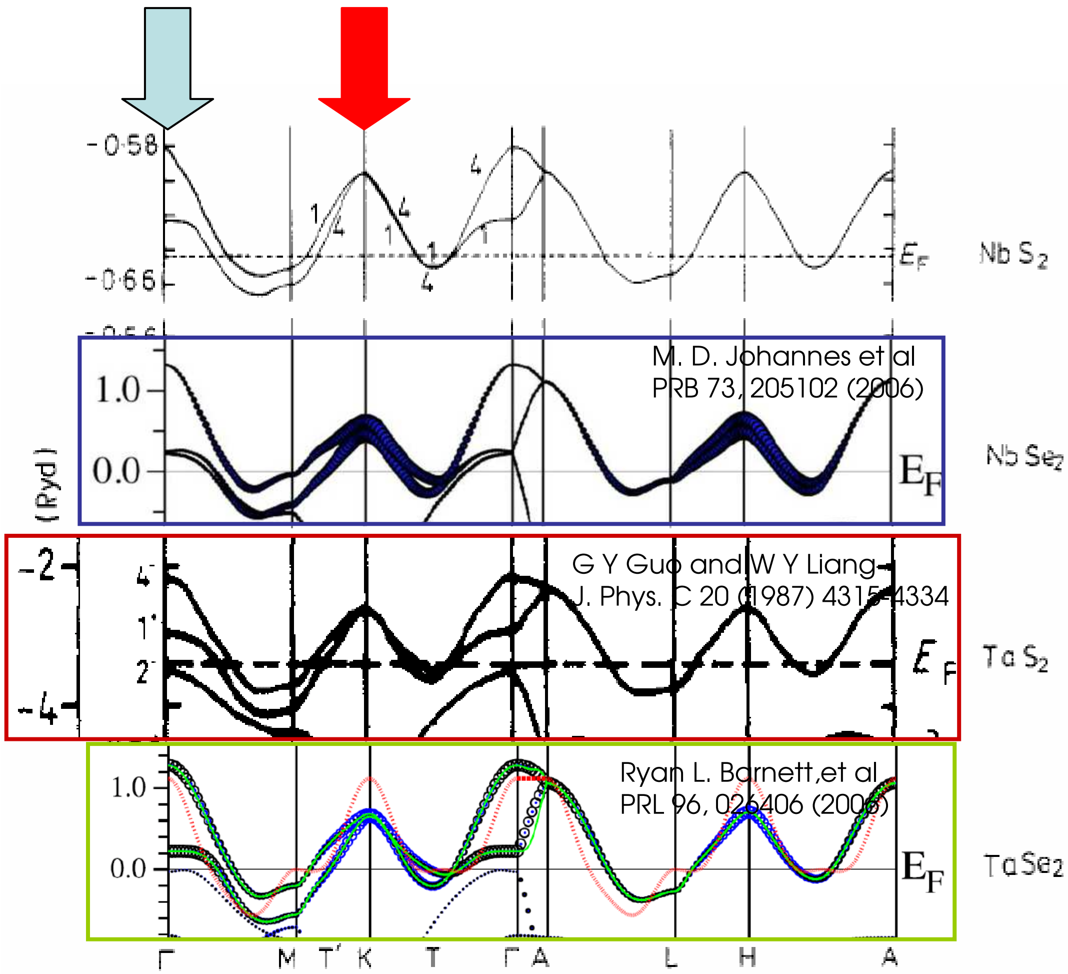
CDW & Fermi Surface in 2H transition metal dichalcogenides



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



G Wexler and A WooleyJ.Phys.C 9, 1185 (1976)

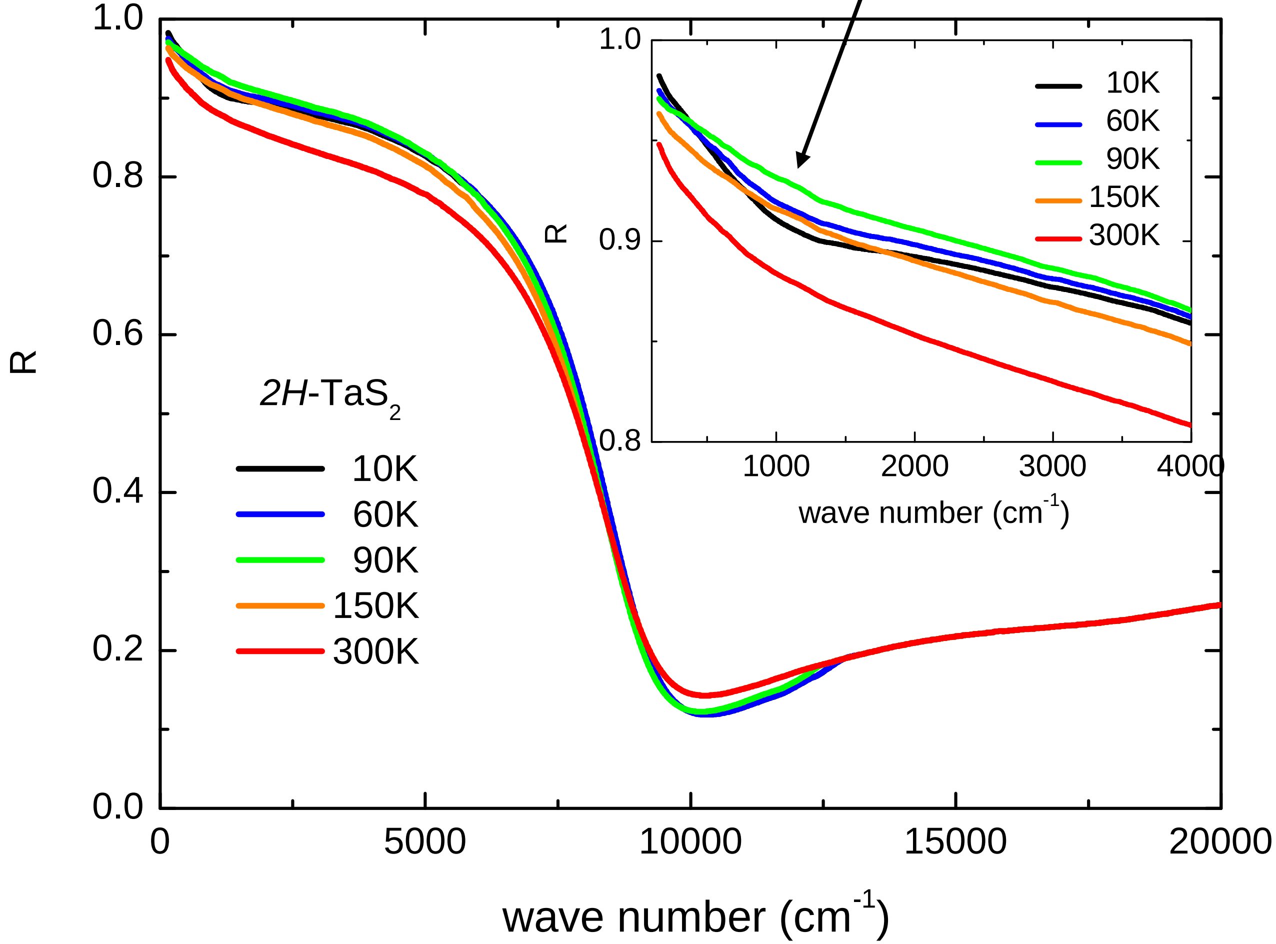


Typical behavior of partial energy gap at Fermi surface in R(ω)

2H-TaS2

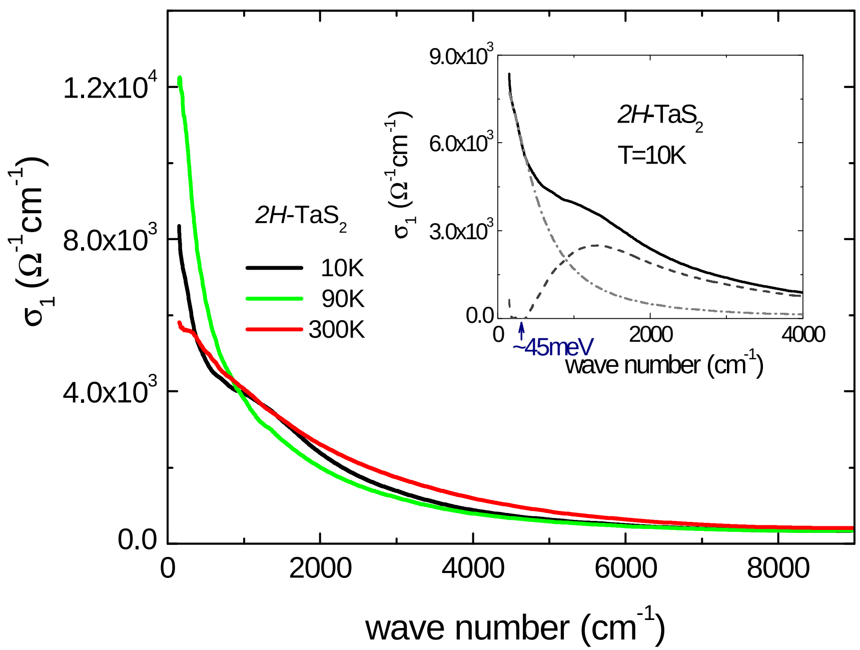
T_{CDW}=75 K

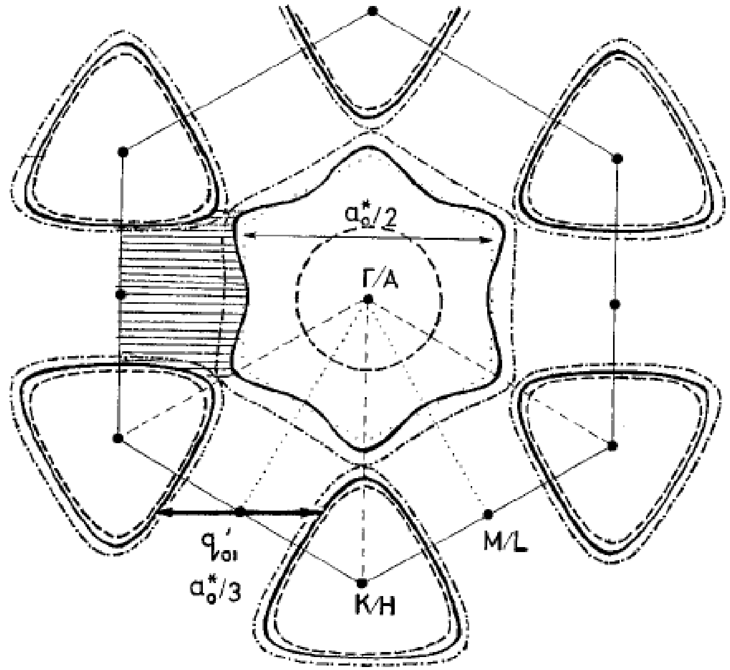
T_c=0.8 K

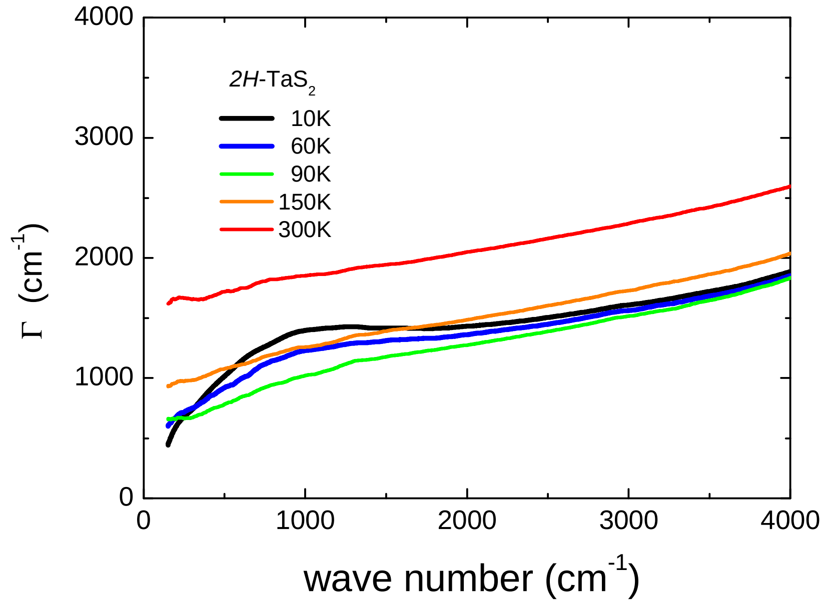


W. Z. Hu et al., PRB (07)

Single crystal from XH Chen's group







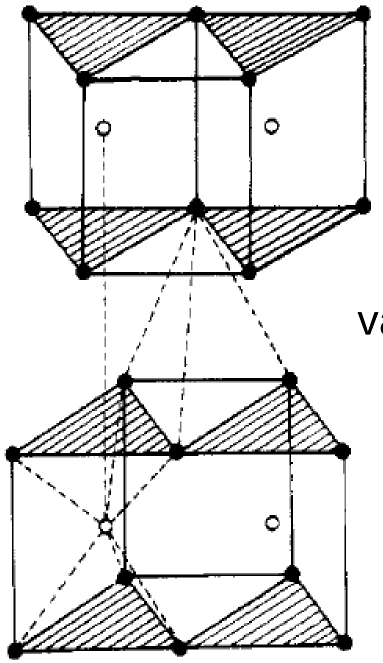
No CDW gap @ Γ pocket, but the K pocket is partially gapped.

$$\Gamma(\omega) = \frac{1}{\tau(\omega)} = \frac{\omega_p^2}{4\pi}\mathrm{Re}\left(\frac{1}{\sigma(\omega)}\right)$$

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

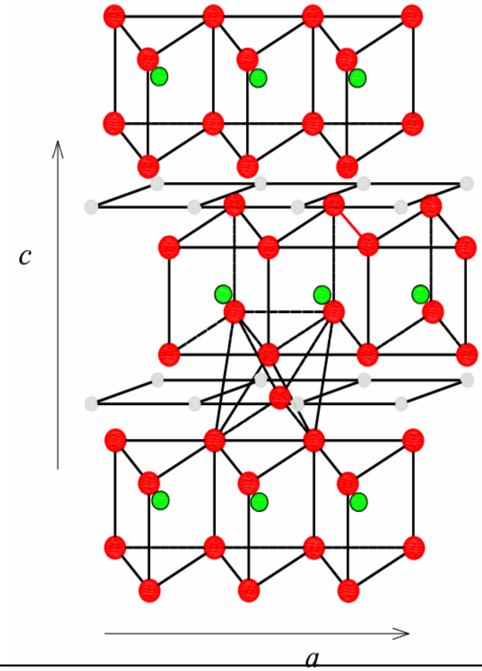
Received 8 August 1975



van der Waals gap

Figure 1. Structure of the 2H-metallic transition-metal dichalcogenides; ● chalcogens, ○ metals.

intercalation

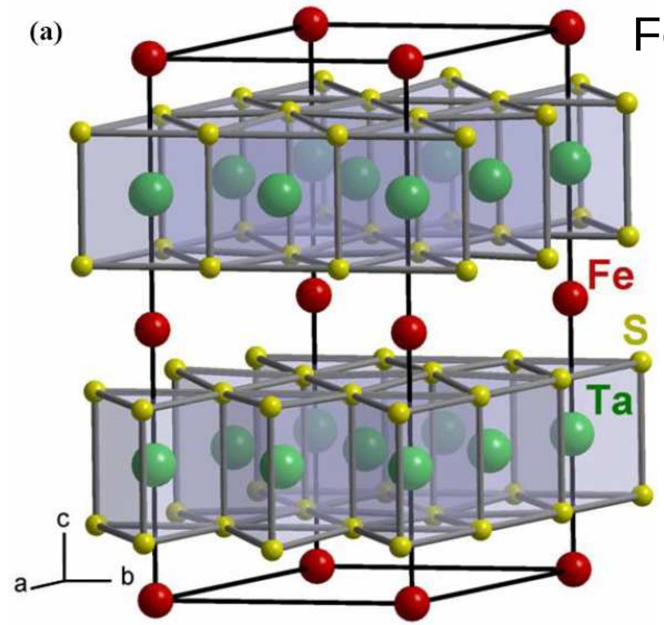


Na_xTaS_2,

Li_xNbO_2,

Cr_xNbSe_2

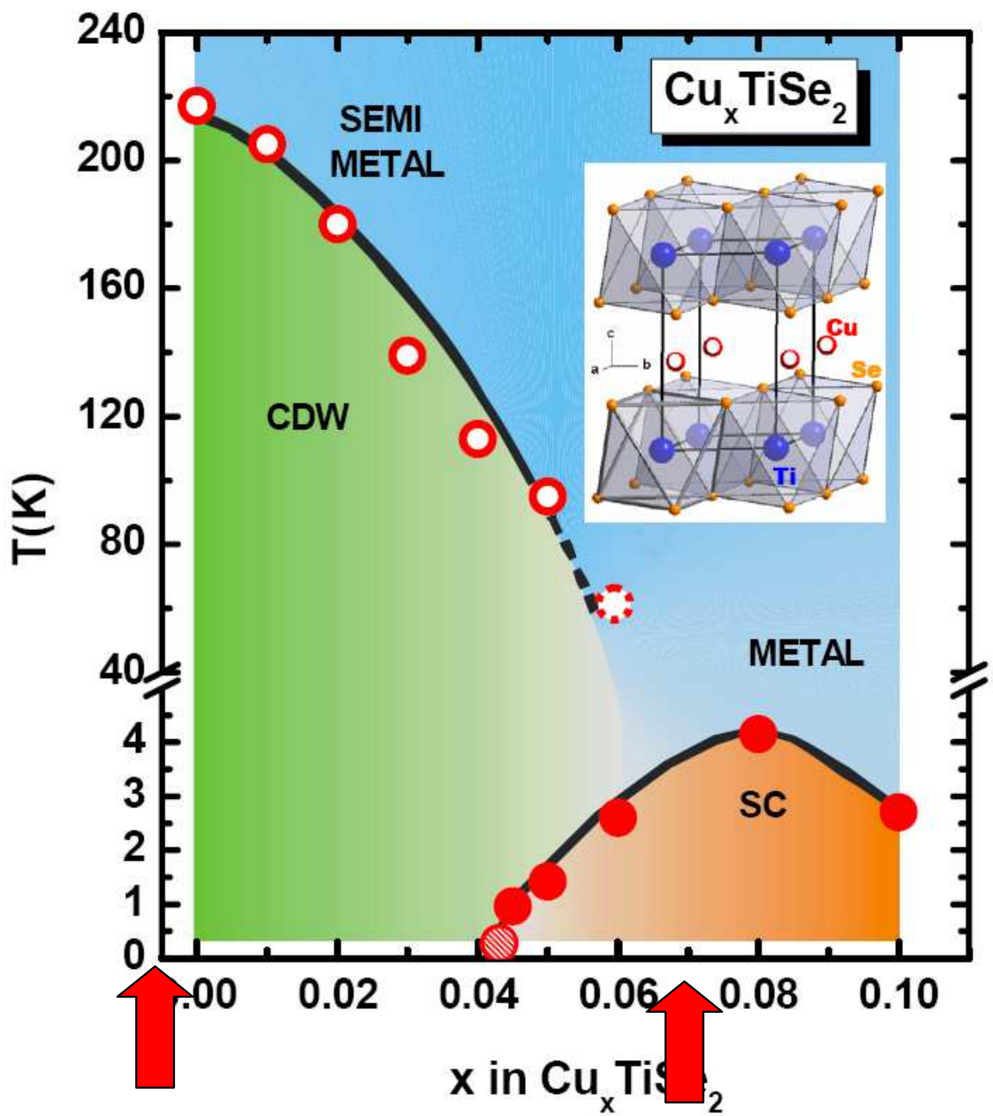
……

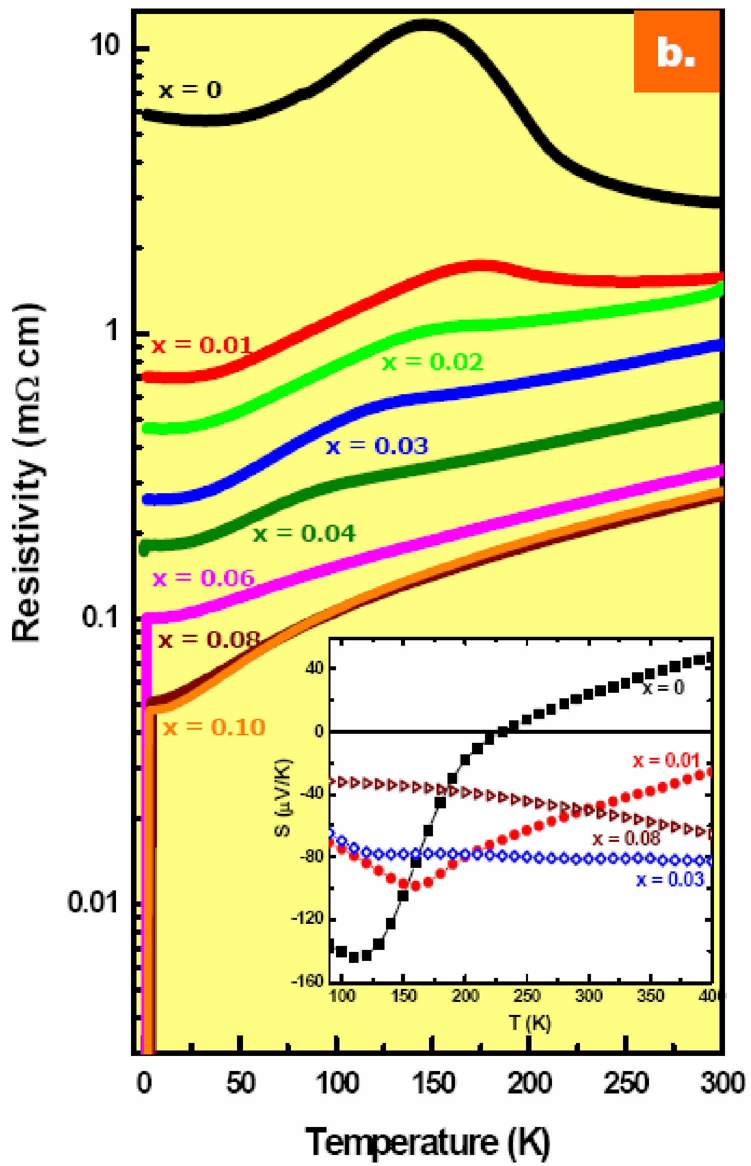


$Fe_{1/4}TaS_2$

E. Morosan et al. cond-mat/0701311

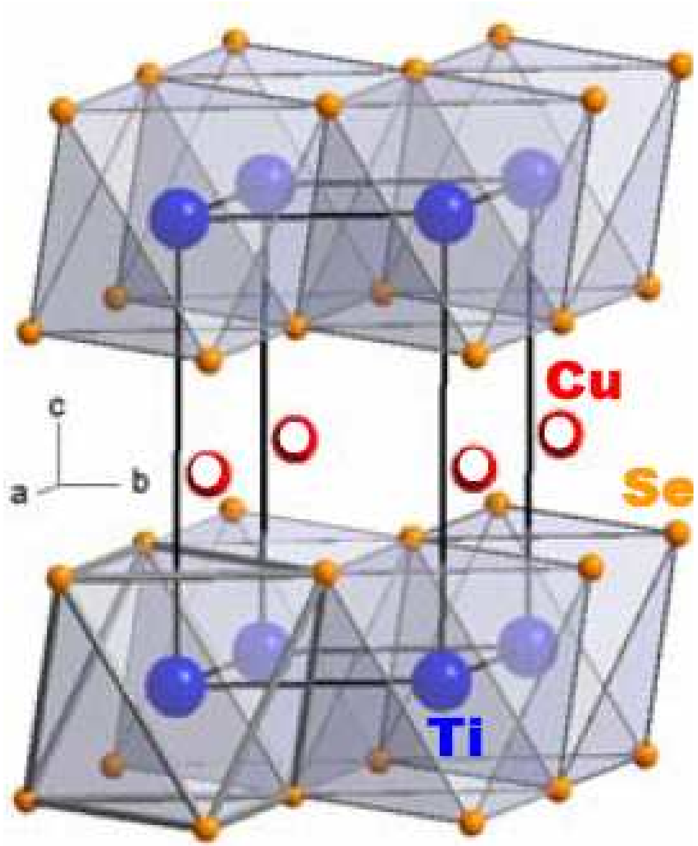
Newly discovered Cu_xTiSe_2





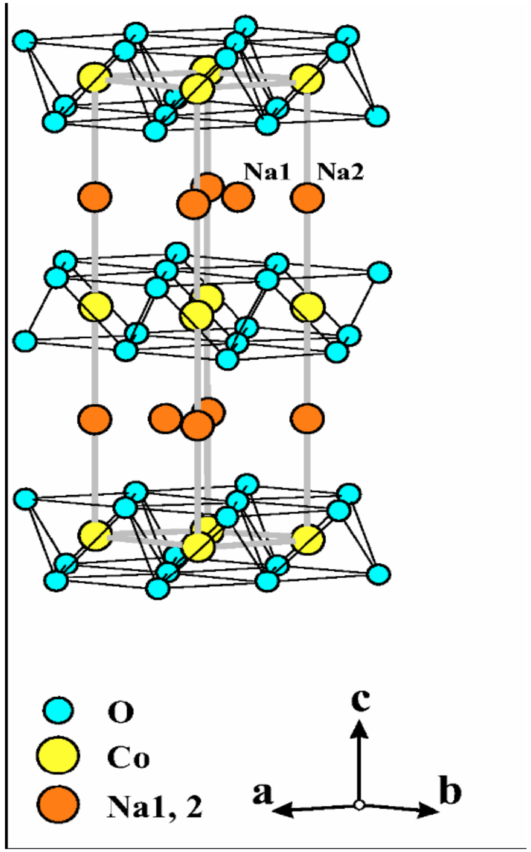
E. Morosan et al, Nature Phys. 06

Only superconductor
with 1T structure



Na_xCoO_2

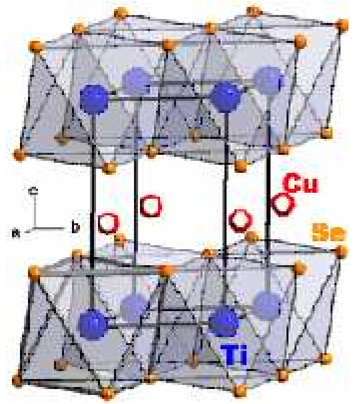
a=2.84 A c=10.81 A,
space group: P6/mmc



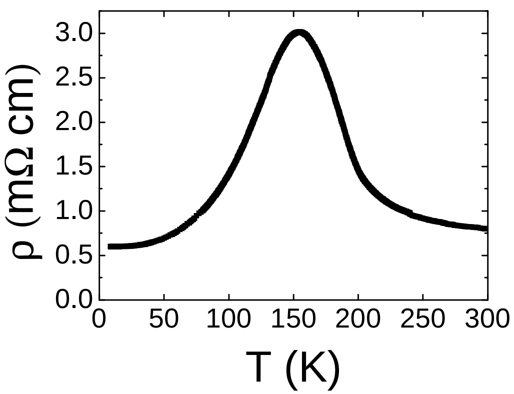
1T+2H structural block

Parent compound 1T-TiSe2

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



- Broken symmetry at 200 K with a 2x2x2 superlattice



PHYSICAL REVIEW B VOLUME 17, NUMBER 4 15 FEBRUARY 1978

Band structure and lattice instability of $TiSe_2$

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(Received 23 June 1977)

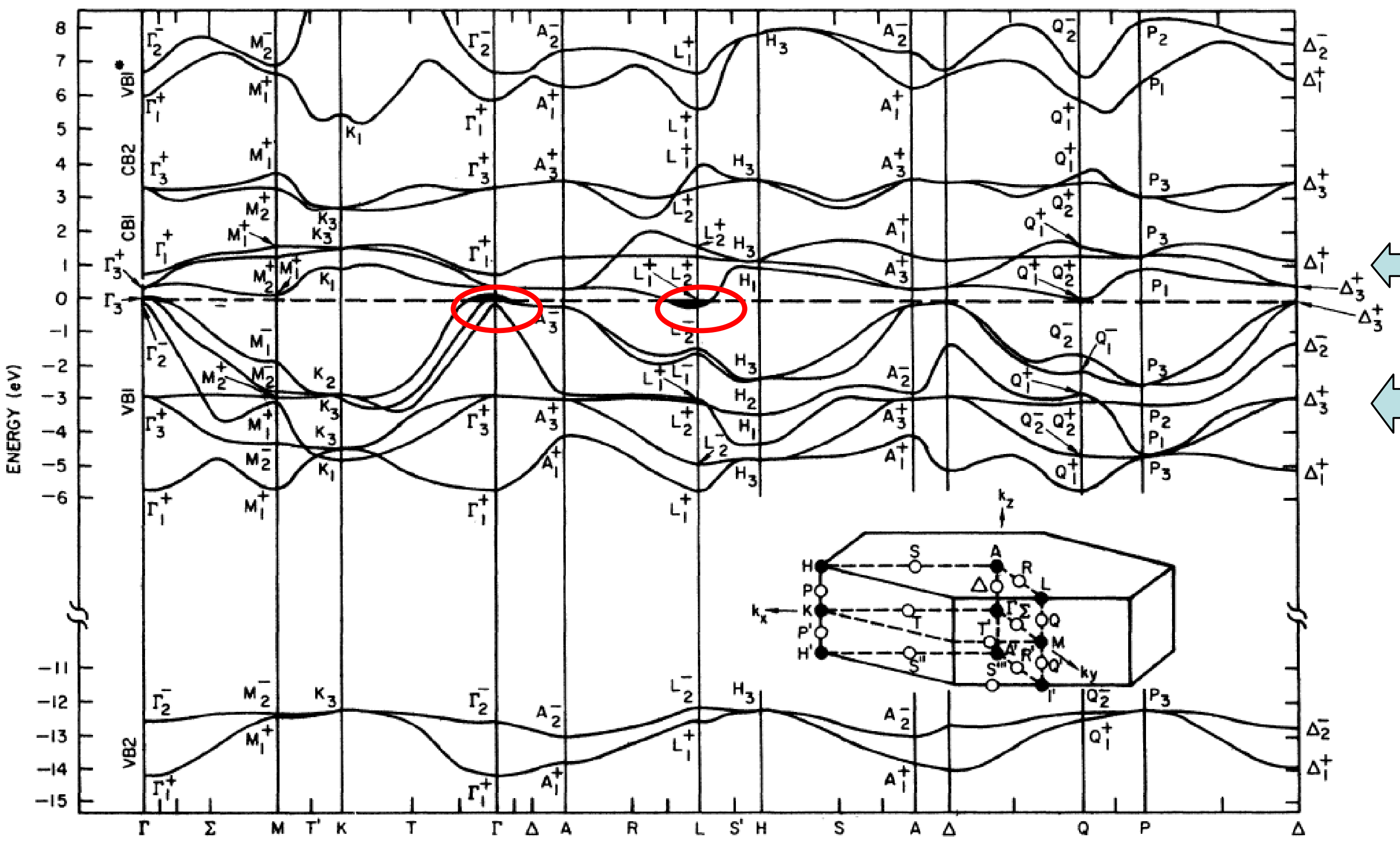

FIG. 1. Energy-band structure of $TiSe_2$ in the local exchange and correlation model.

Ti: $3d^24s^2$

Se: $4s^24p^4$

Ti : 3d band

Se: 4p band

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

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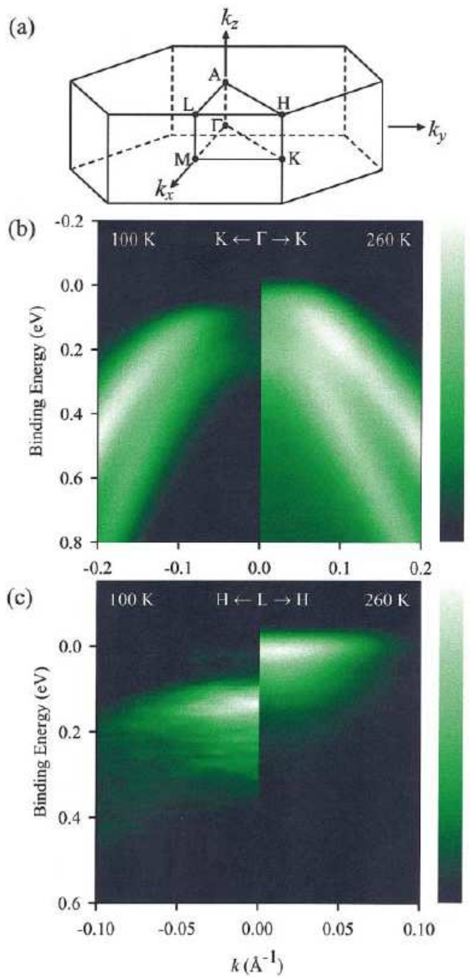
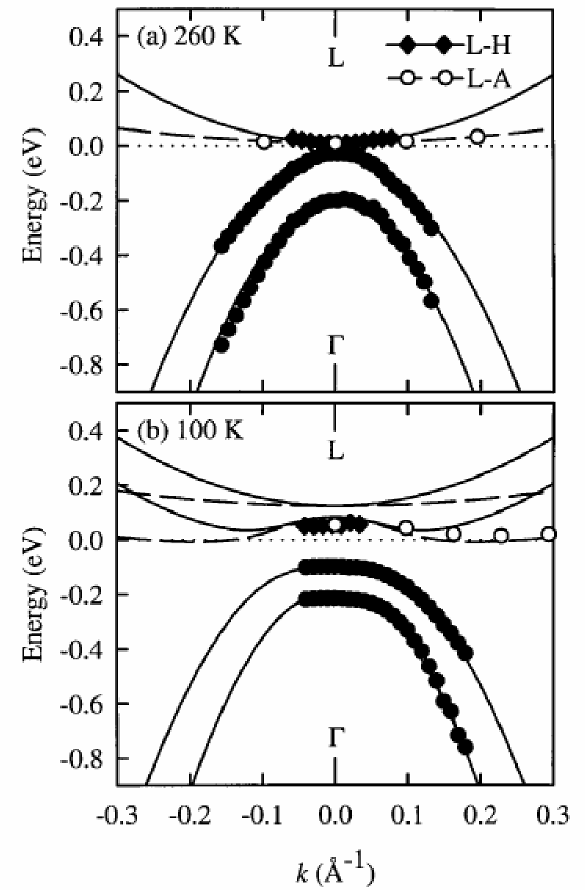
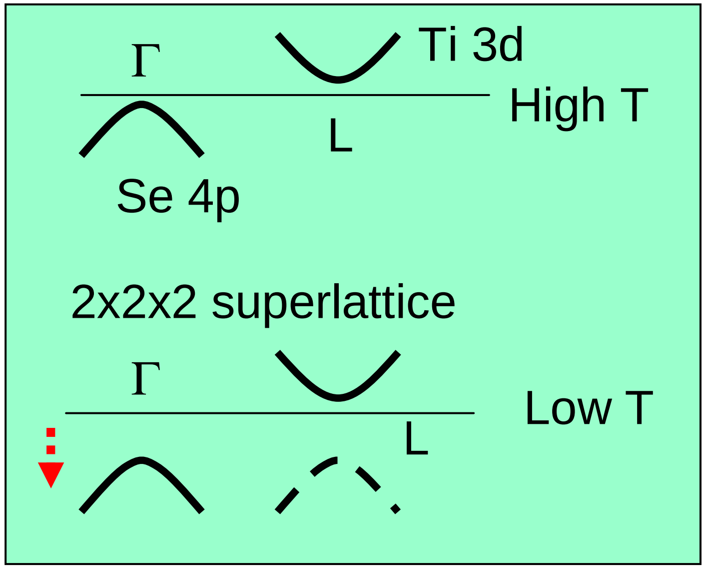
and Frederick Seitz Materials Research Laboratory, University of Illinois at Urbana-Champaign, 104 South Goodwin Avenue, Urbana, Illinois 61801-2902
[2]*School of Physics, Georgia Institute of Technology, Atlanta, Georgia 30332-0430*
(Received 8 November 2001; published 17 May 2002)





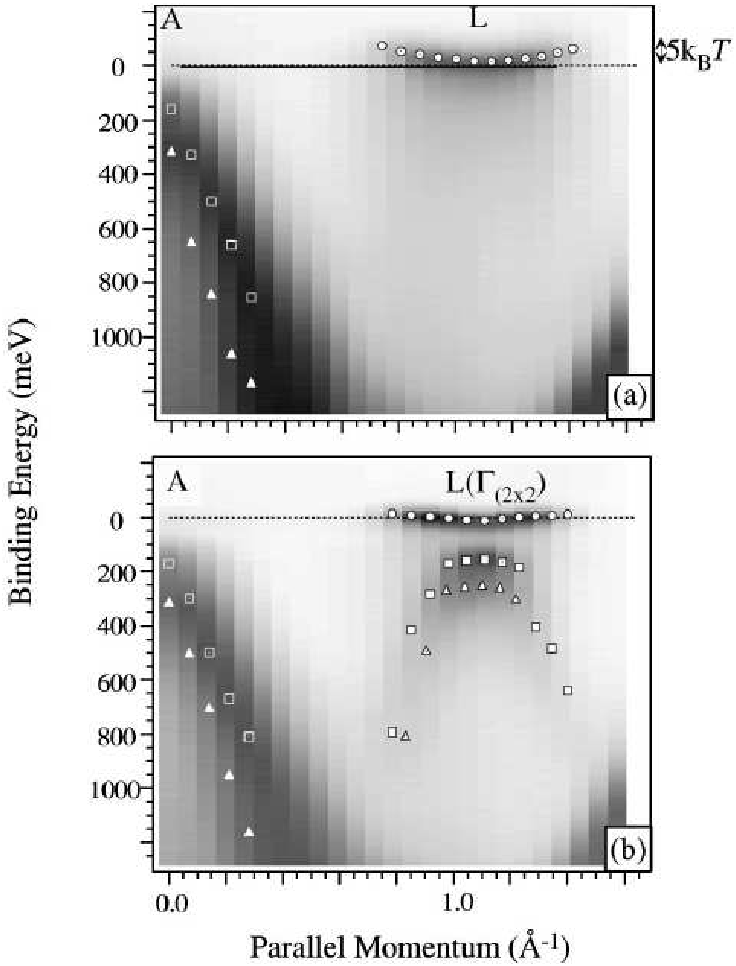


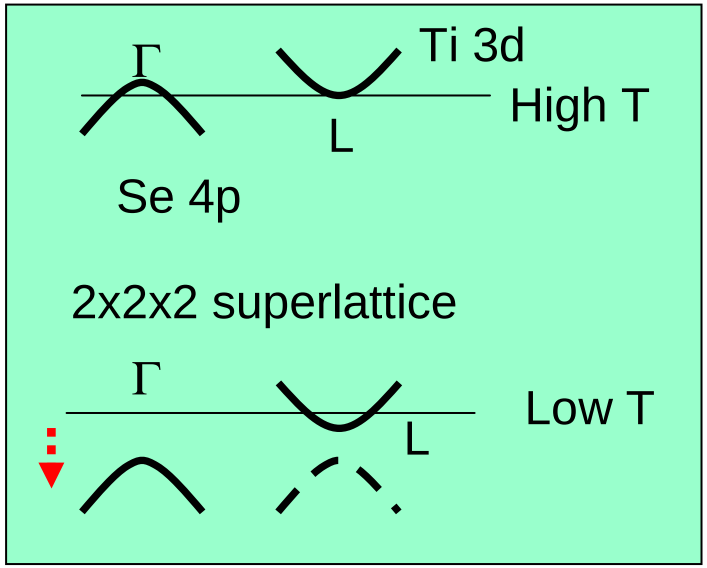
No band crossing
Fermi level below CDW.

It is insulating!!

Photoemission of bands above the Fermi level: The excitonic insulator phase transition in 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.

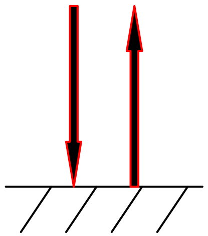
- The mechanism of the CDW transition:

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

Optical measurement

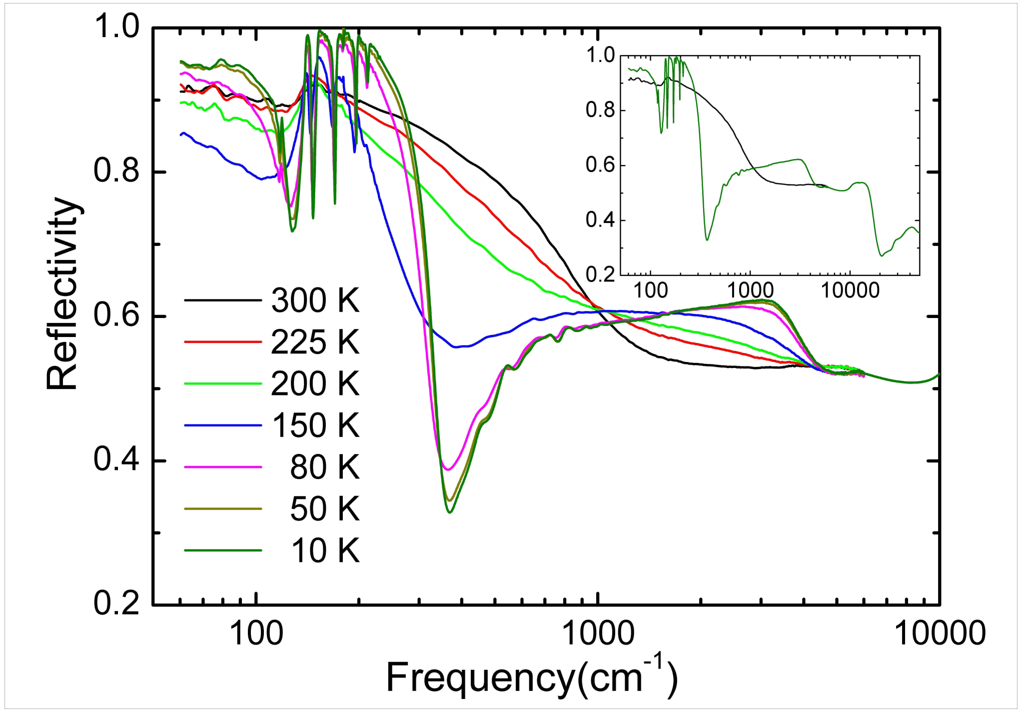
Experiment:

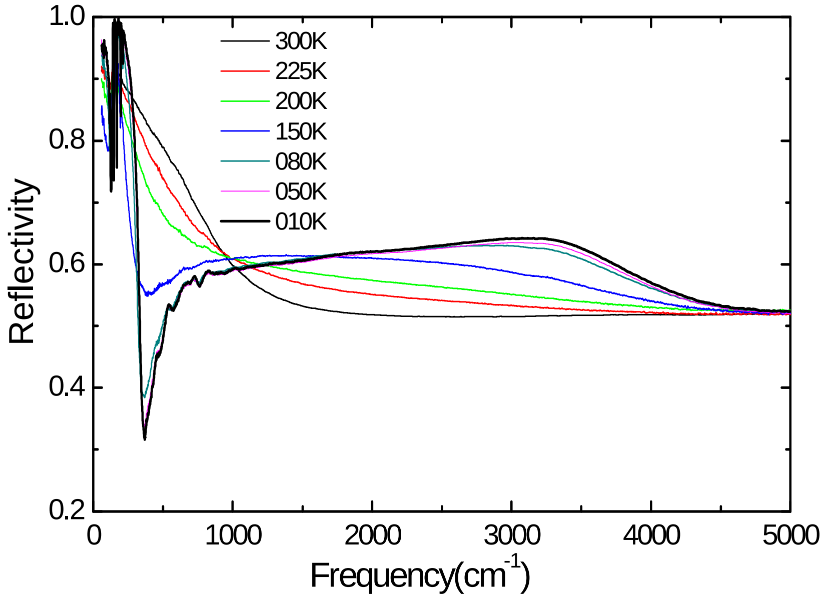
Reflectivity R(ω)

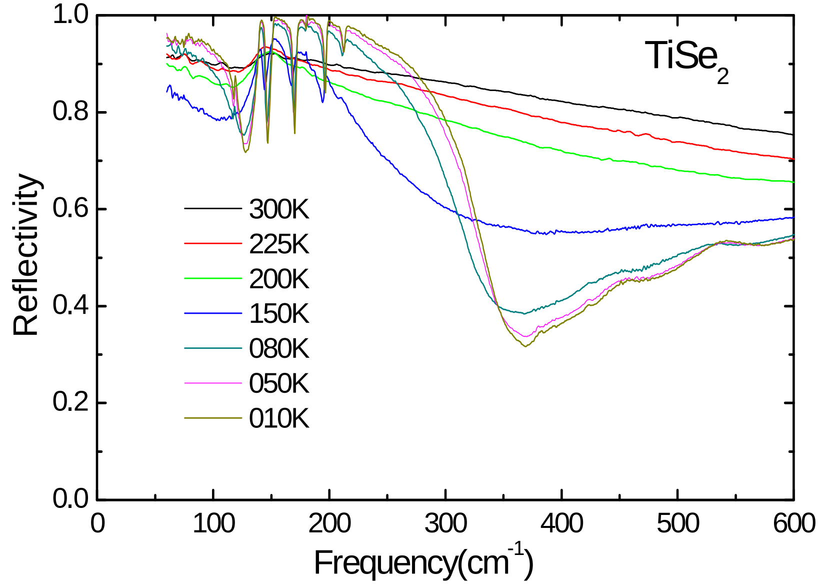


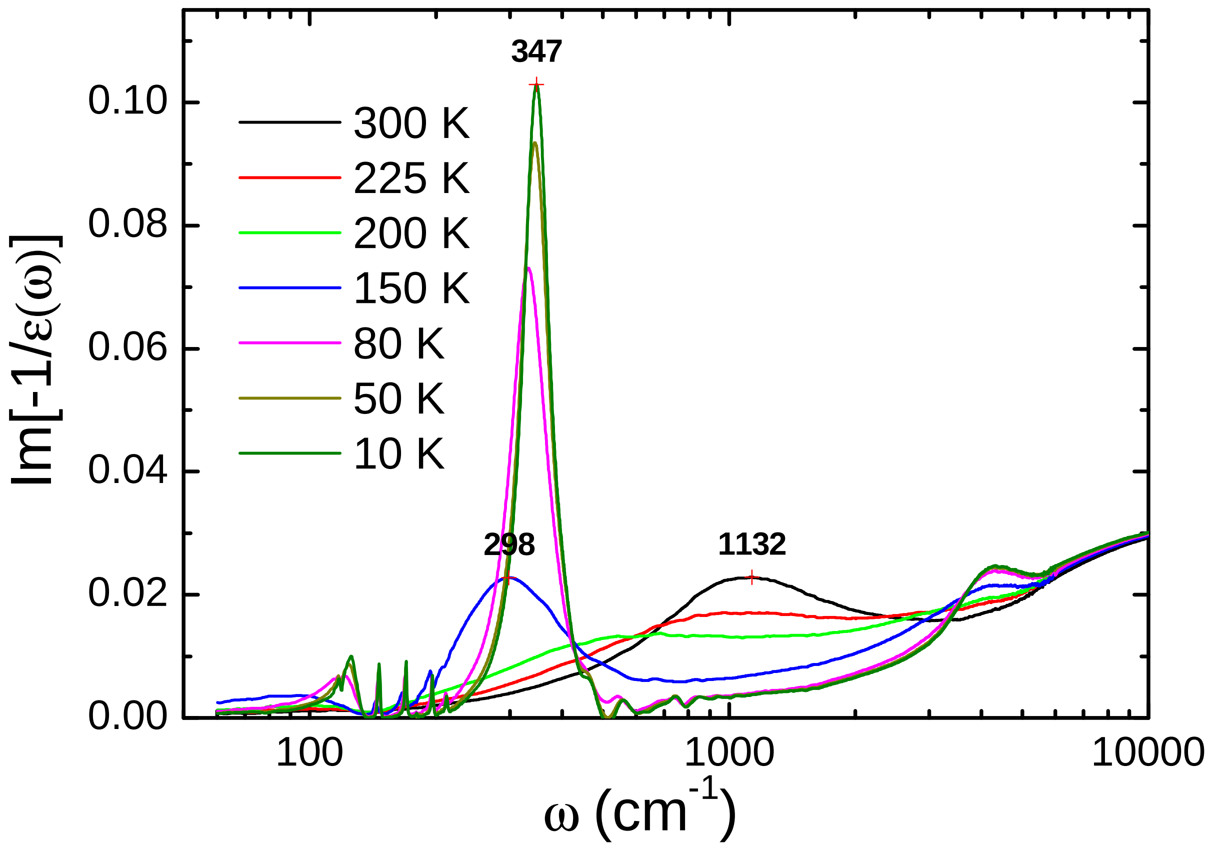
$TiSe_2$ single crystal

G. Li et al., PRL (07a)

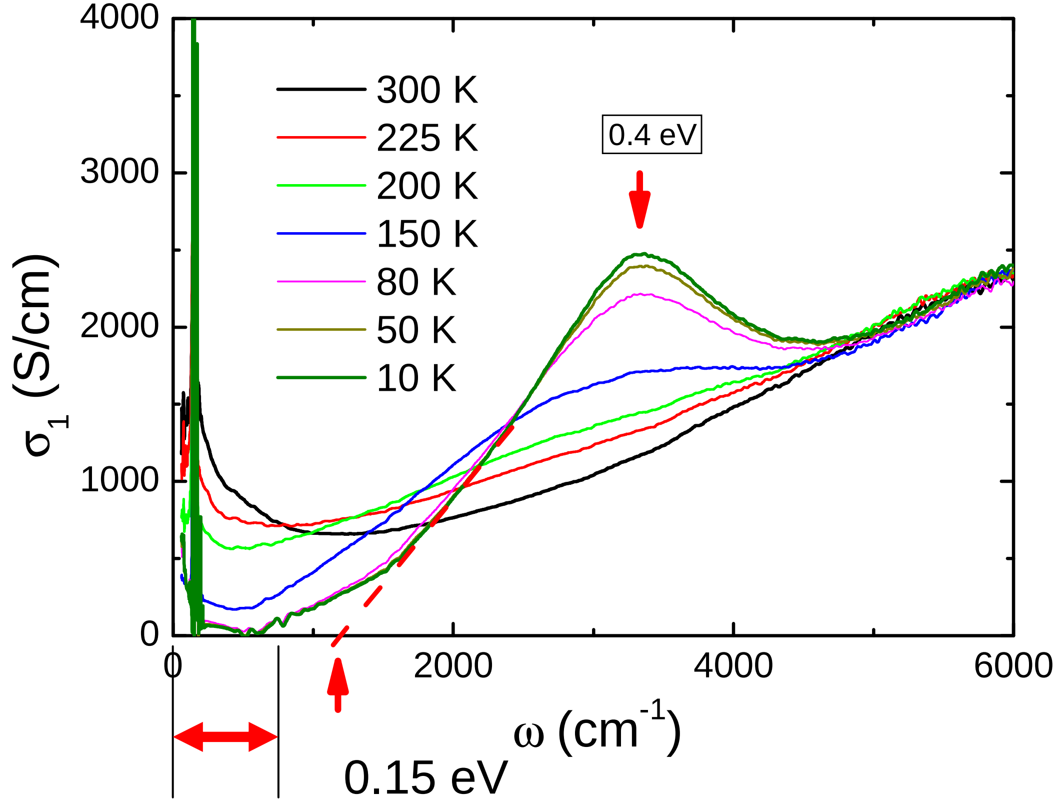




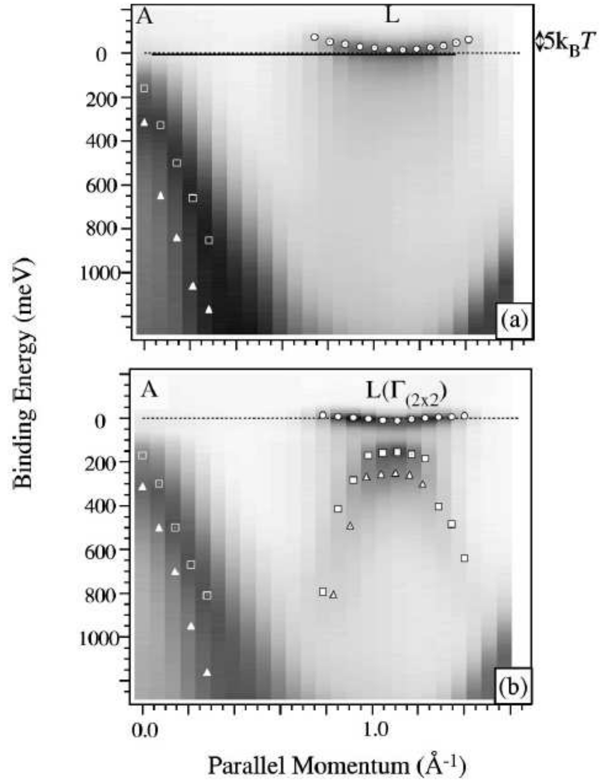




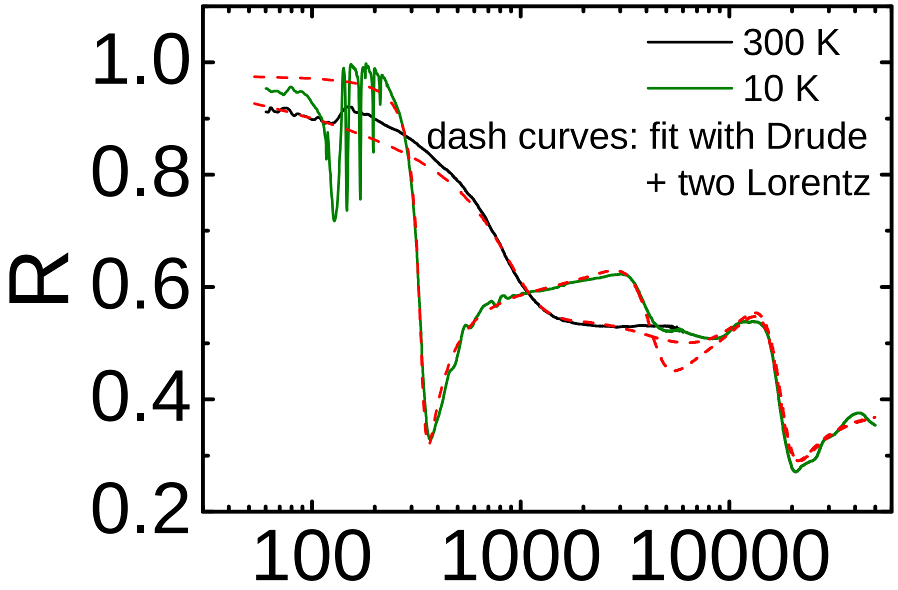
$$\omega_p' = \omega_p / \sqrt{\varepsilon_\infty}$$

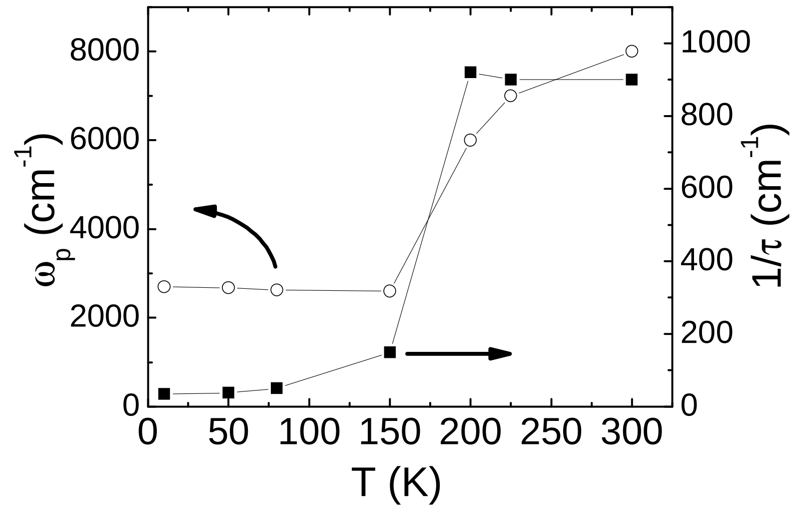


Drude CDW gap



Free carriers with very long relaxation time exist in the CDW gapped state ⇨ FS is not fully gapped??





$$\epsilon(\omega) = \epsilon_\infty - \frac{\omega_p^2}{\omega^2 + i\omega/\tau} + \sum_{i=1}^{2} \frac{S_i^2}{\omega_i^2 - \omega^2 - i\omega/\tau_i}. \qquad (1)$$

It contains a Drude term and two Lorentz terms, which approximately capture the contributions by free carriers and interband transitions. As shown in the inset of

Semimetal to semimetal transition for CDW

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

- Carrier density changes with T, decreases from room T to 150 K then increases slightly with further decreasing T

- Development of an energy gap ~0.15 eV below 200 K

- Dramatic different carrier damping at different T

Excitonic Phases W. Kohn, PRL 67

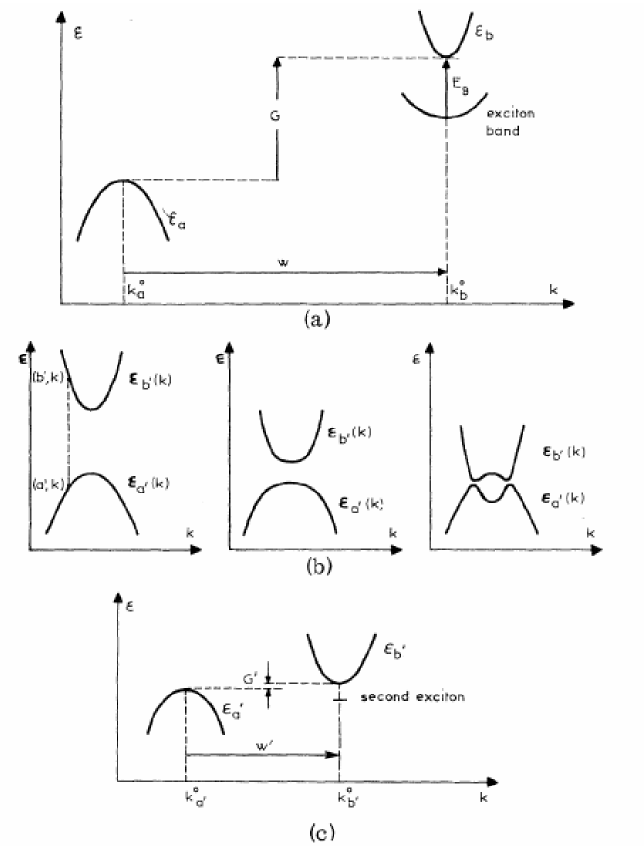


FIG. 1. The insulating side. (a) Energy bands and exciton band of the normal insulator. (b) The new energy bands after the first excitonic transition for successive values of the external parameter (e.g., pressure). (c) The second excitonic instability.

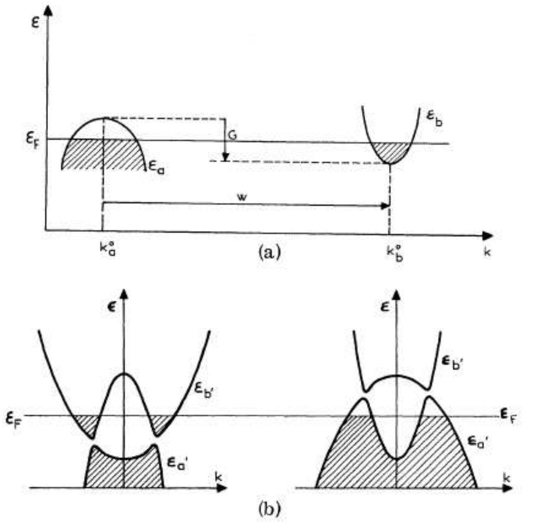


FIG. 2. The metallic side. (a) Energy bands of the normal semimetal. (b) Energy bands after the first Overhauser transition for two different directions of k.

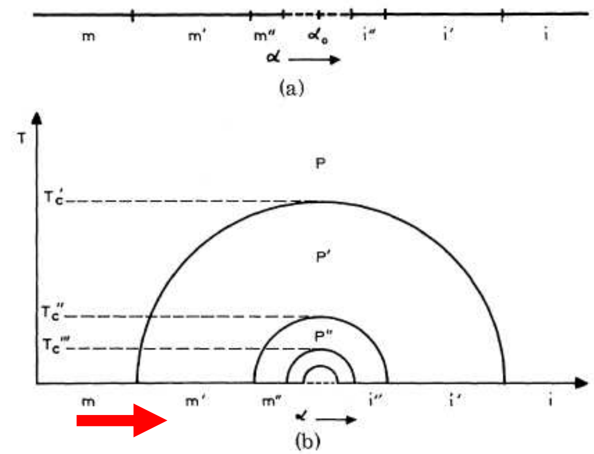
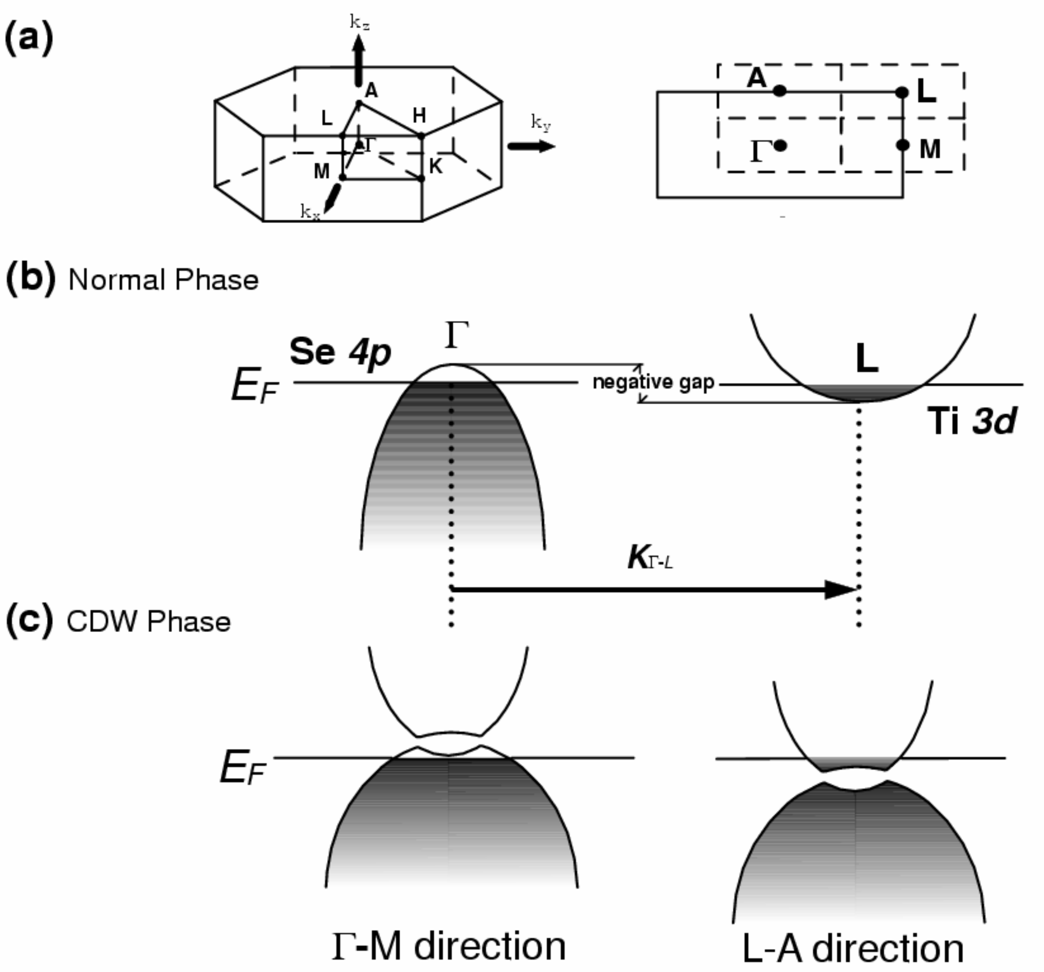
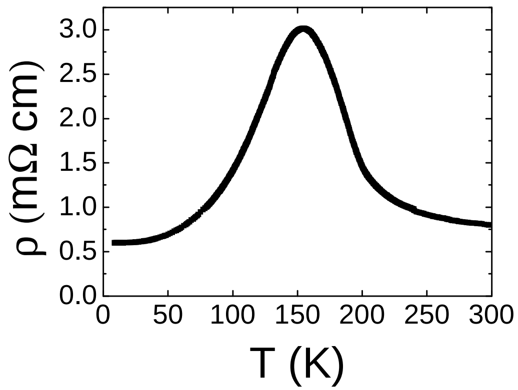


FIG. 3. The excitonic phases. (a) Succession of phases, at $T=0°$, for different values of α; m, metallic; i, insulating. The dotted interval contains an infinity of m and i phases. (b) Total phase diagram, showing an infinity of nested phases.

The electron-hole coupling acts to mix the electron band and hole band that are connected by a particular wave vector.





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

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

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

Exciton-driven CDW

G. Li et al., PRL (07a)

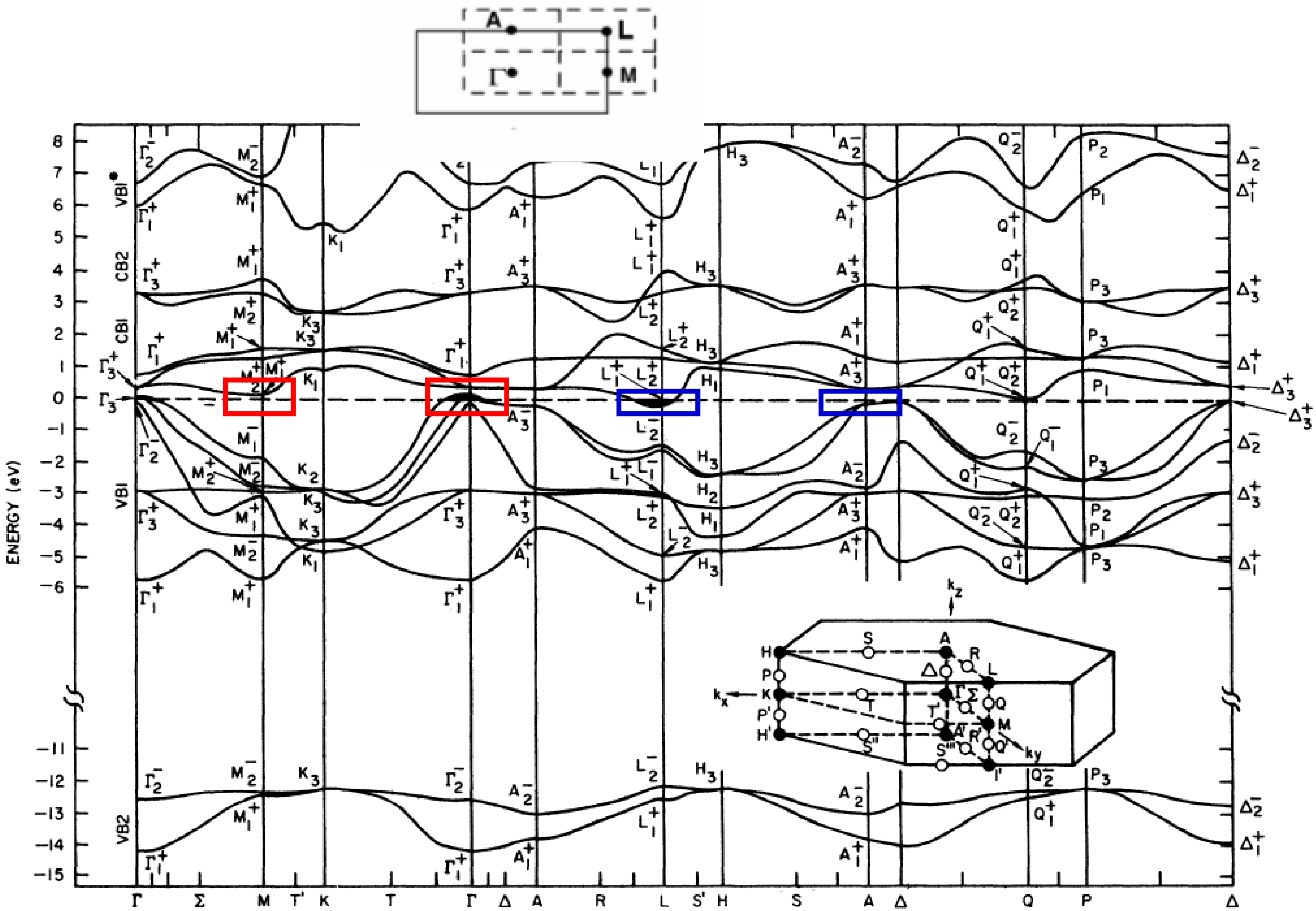
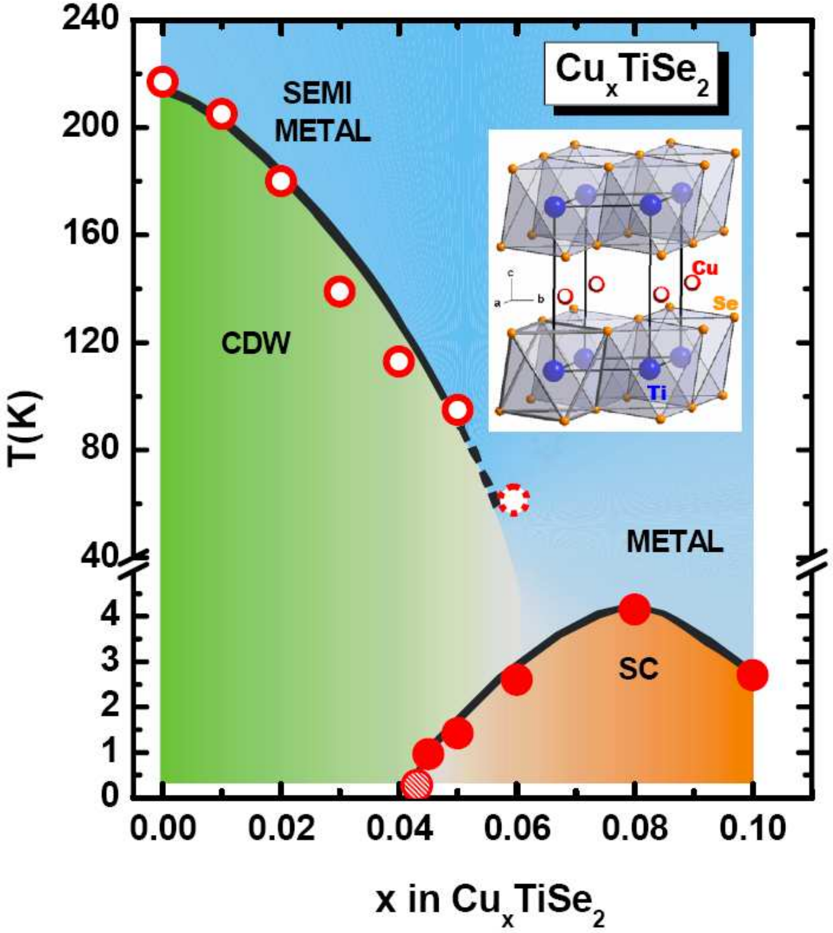
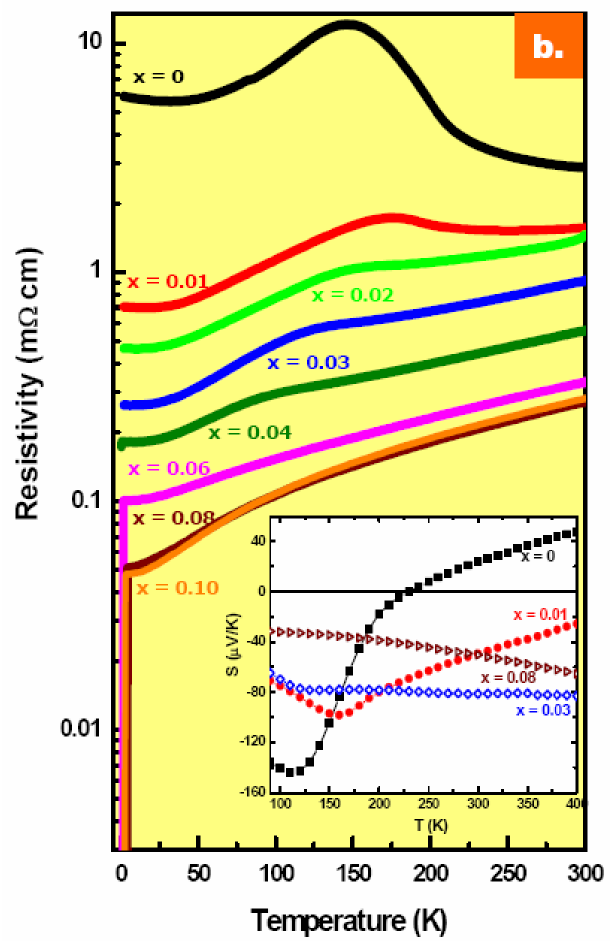
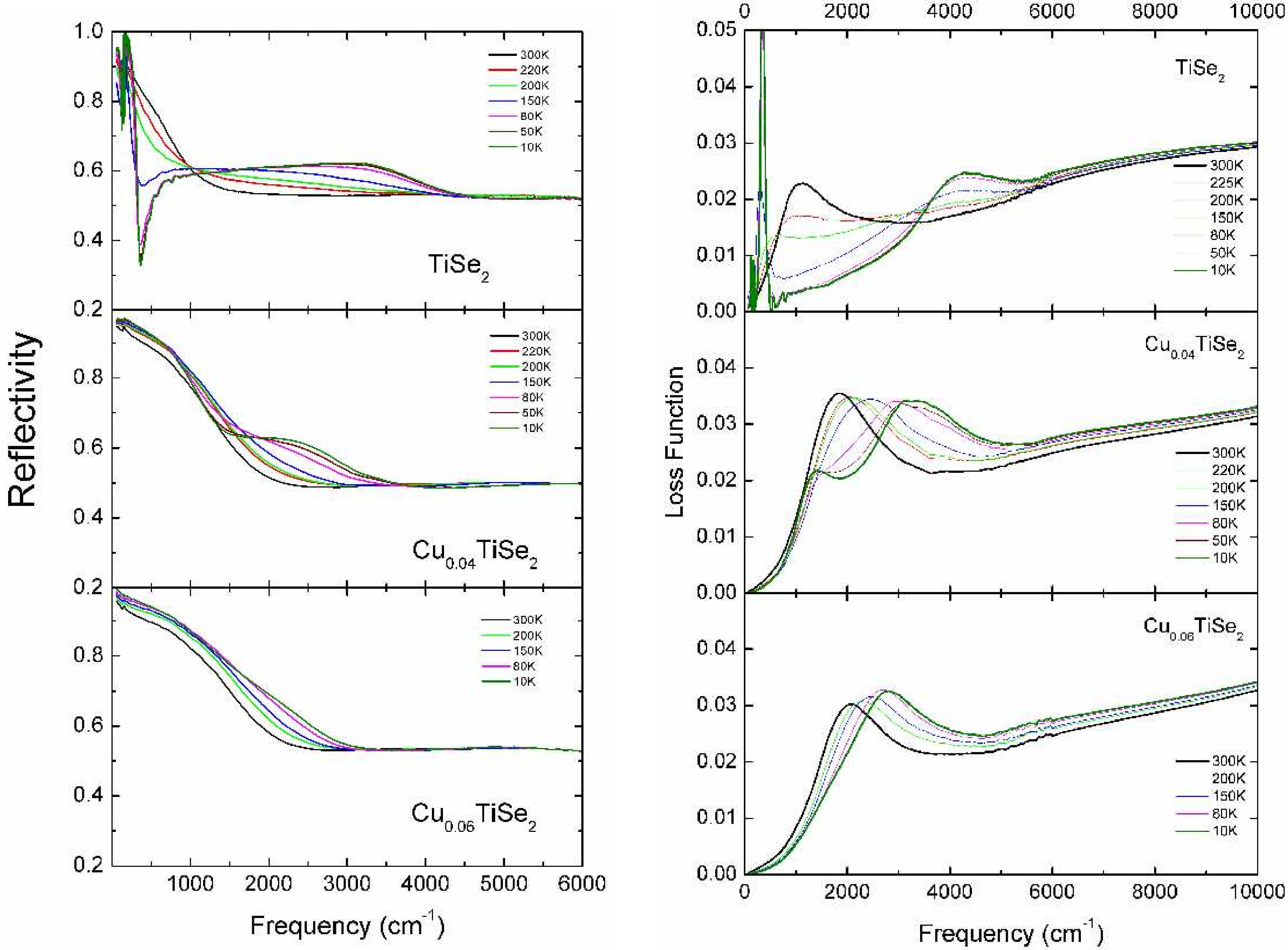


FIG. 1. Energy-band structure of $TiSe_2$ in the local exchange and correlation model.

Cu-doped CuxTiSe2

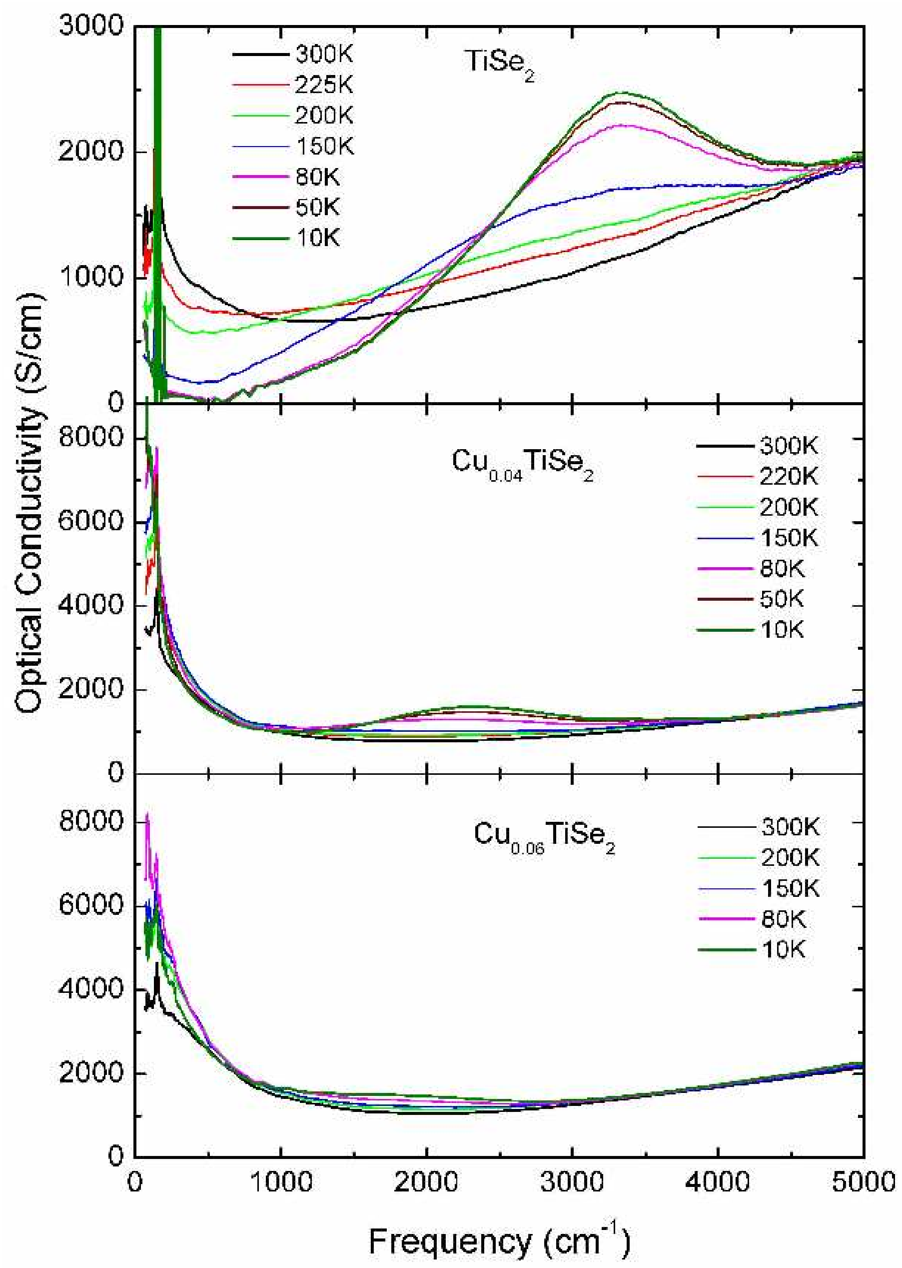


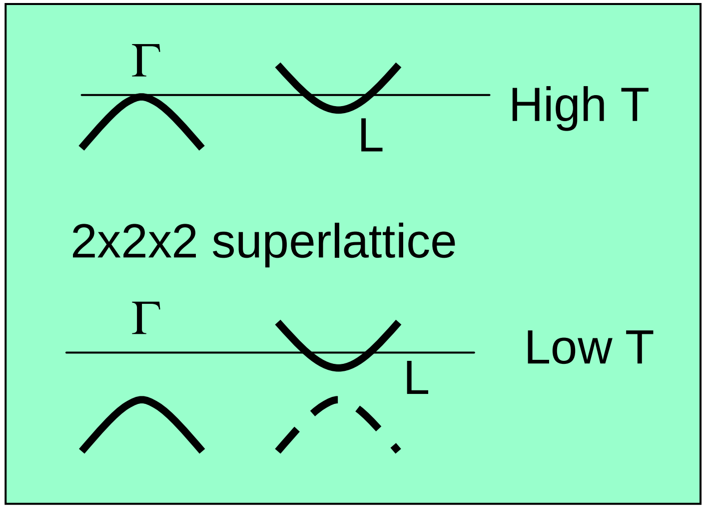




Reflectivity
TiSe2
Cu0.04TiSe2
Cu0.06TiSe2
300K
220K
200K
150K
80K
50K
10K
Frequency (cm-1)
Loss Function
225K

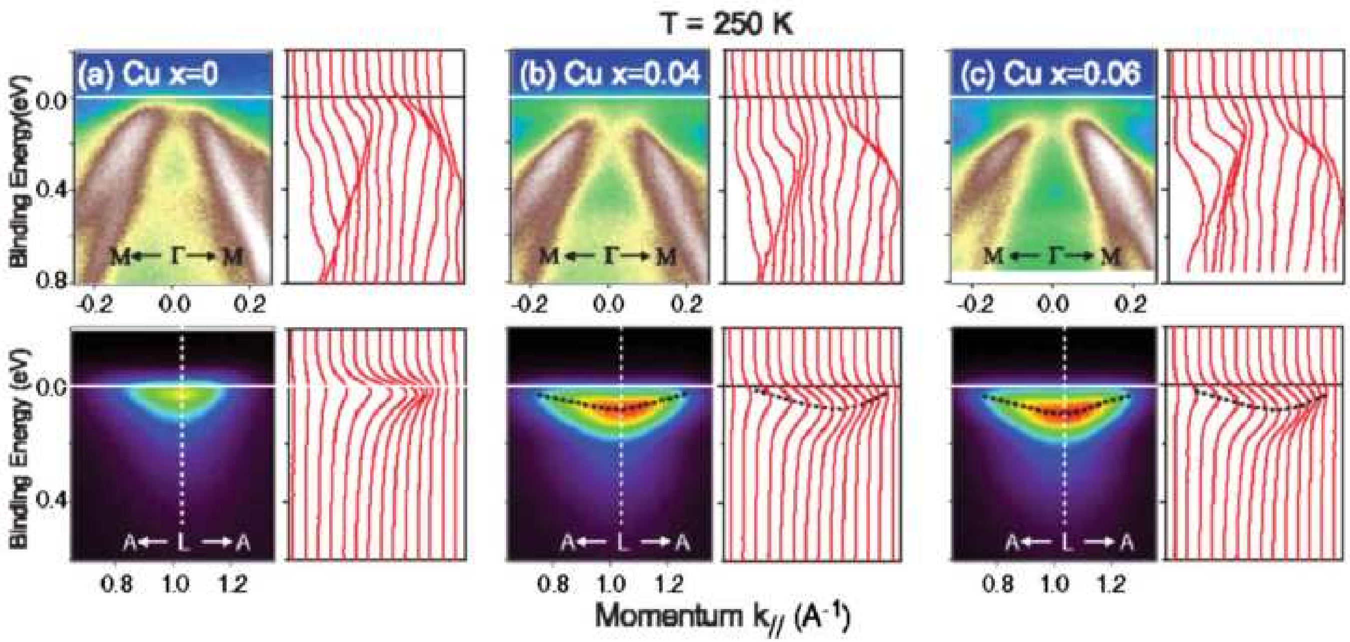
CDW gap still exists





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

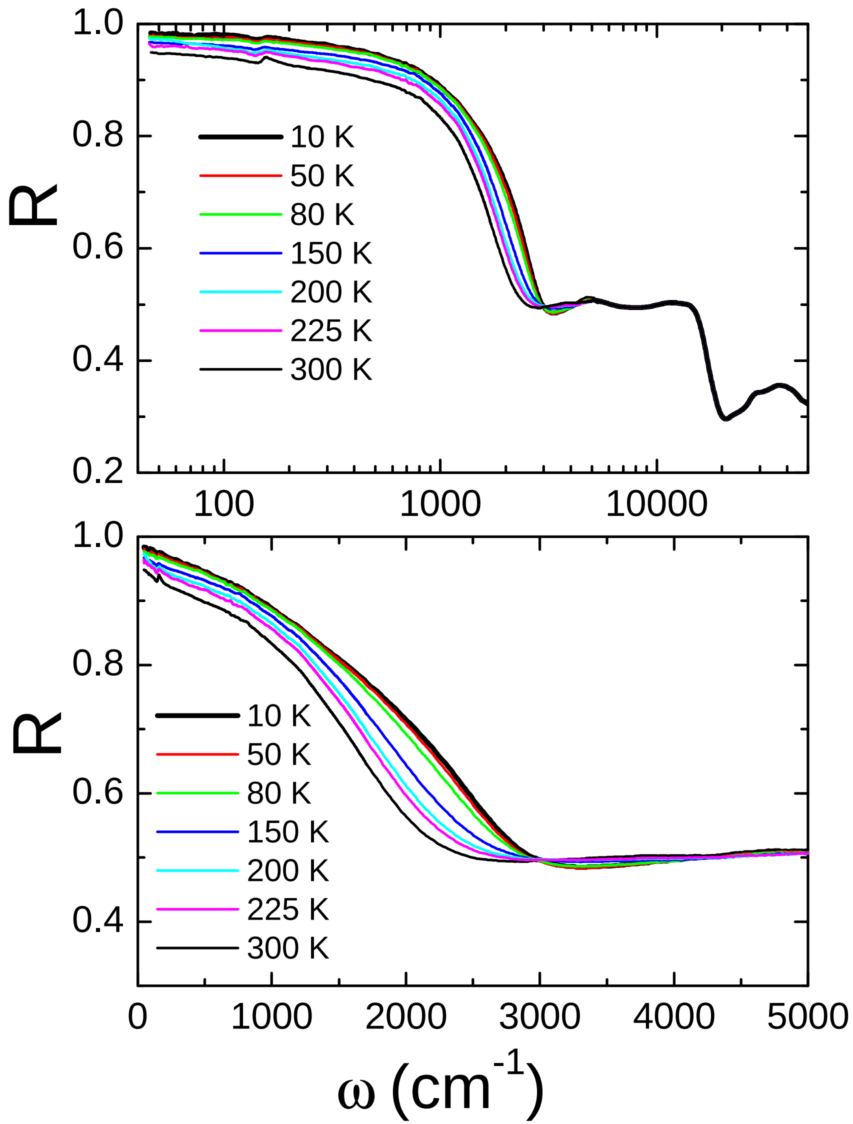
D. Qian,[1] D. Hsieh,[1] L. Wray,[1] E. Morosan,[2] N. L. Wang,[3] Y. Xia,[1] R. J. Cava,[2] and M. Z. Hasan[1,4,*]

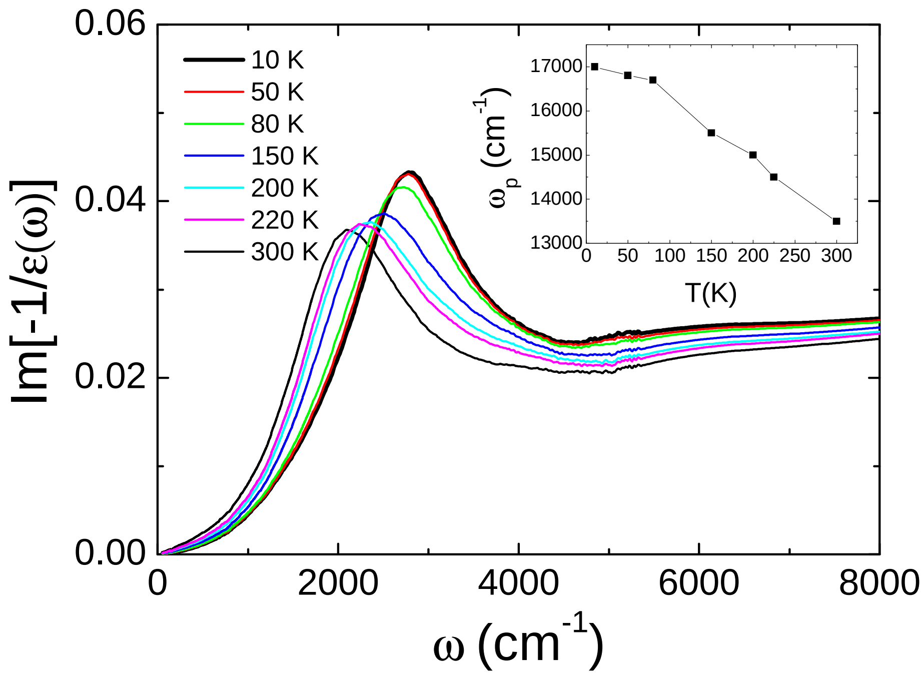


Single band metal

X=0.07

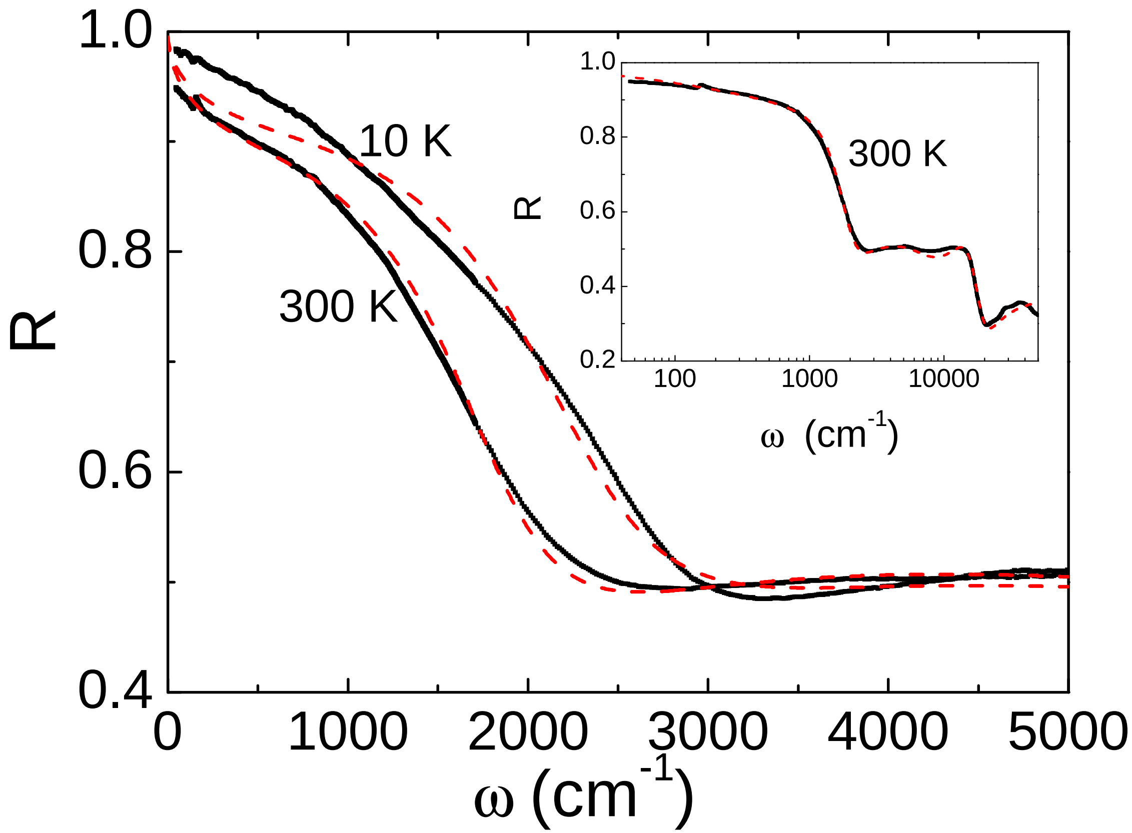
G. Li et al., PRL (07b)





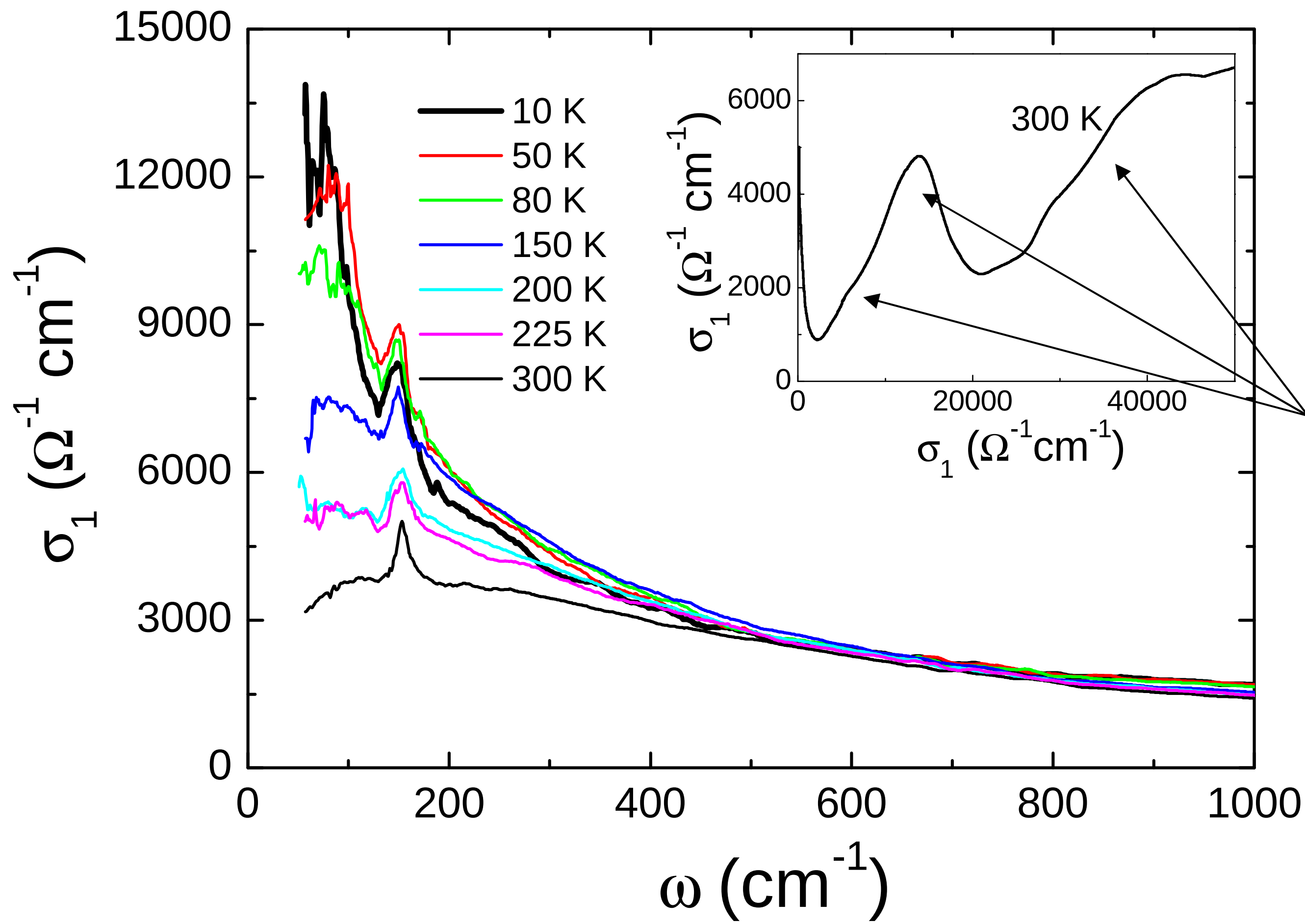
Plasma frequency increases with decreasing T!!

Rarely seen phenomenon!!



$$\epsilon(\omega) = \epsilon_\infty - \frac{\omega_p^2}{\omega^2 + i\omega/\tau} + \sum_{i=1}^{2} \frac{S_i^2}{\omega_i^2 - \omega^2 - i\omega/\tau_i}. \quad (1)$$

It contains a Drude term and two Lorentz terms, which approximately capture the contributions by free carriers and interband transitions. As shown in the inset of



Interband transitions from Se 4p band to unoccupied part of Ti 3d band

Plasma frequency increases with decreasing T??

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

In terms of two bands:

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

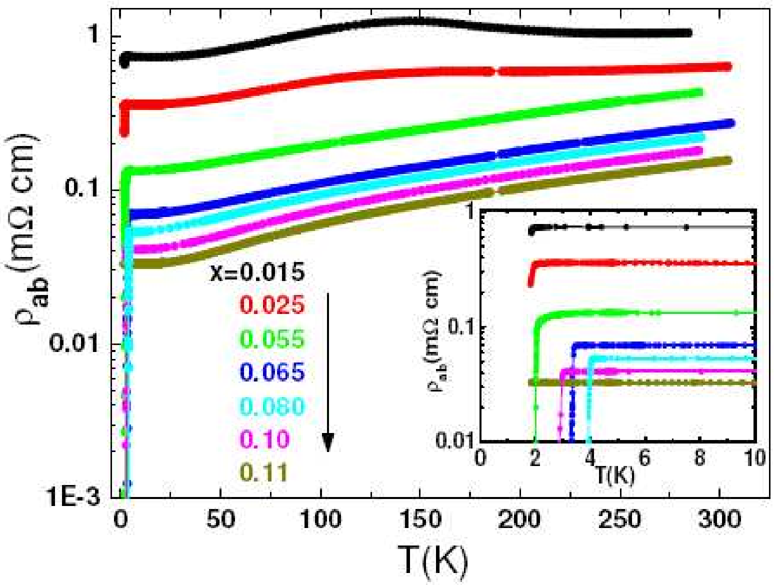
- n increases with decreasing T??

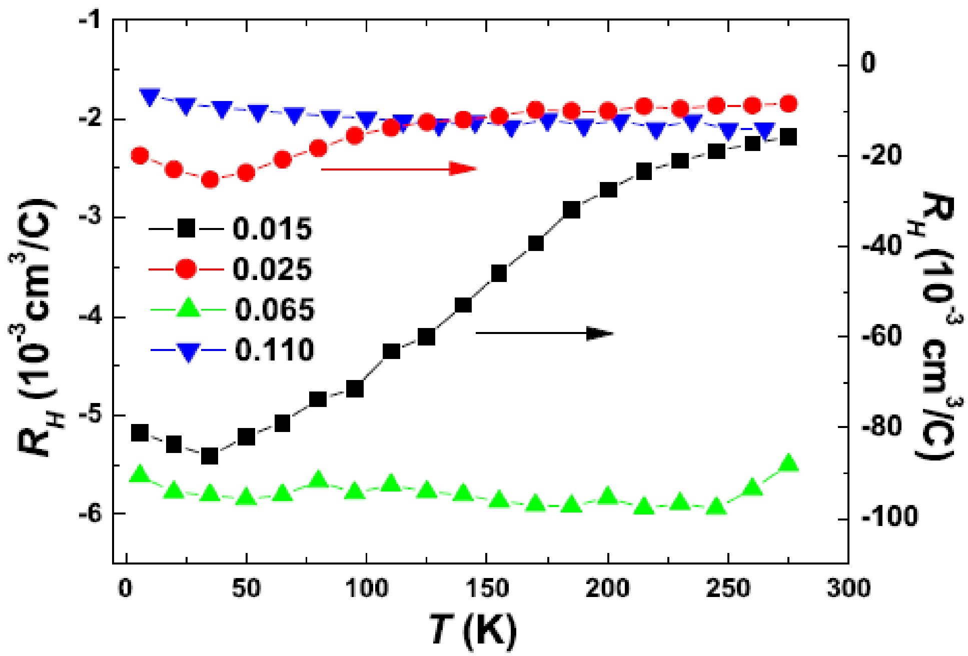
- m* decreases with decreasing T, undressing effect??

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, PRB (07)





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

T-dependent electron-phonon interacton

PHYSICAL REVIEW B VOLUME 1, NUMBER 4 15 FEBRUARY 1970

Temperature Dependence of the Cyclotron Effective Mass in Zinc*

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with a quadratic Fermi surface. As a typical example, for $\omega_{rf}\tau$ of 40 at 4.2°K and 10 at 11°K, the increase in the measured mass would be

$$m^*(11°\text{K}) - m^*(4.2°\text{K}) = 0.0013 m_0^*,$$

where m_0^* is the effective mass for an infinite relaxation time. These very small corrections were applied to the

PHYSICAL REVIEW B VOLUME 1, NUMBER 4 15 FEBRUARY 1970

Calculation of the Temperature Dependence of the Electron-Phonon Mass Enhancement*

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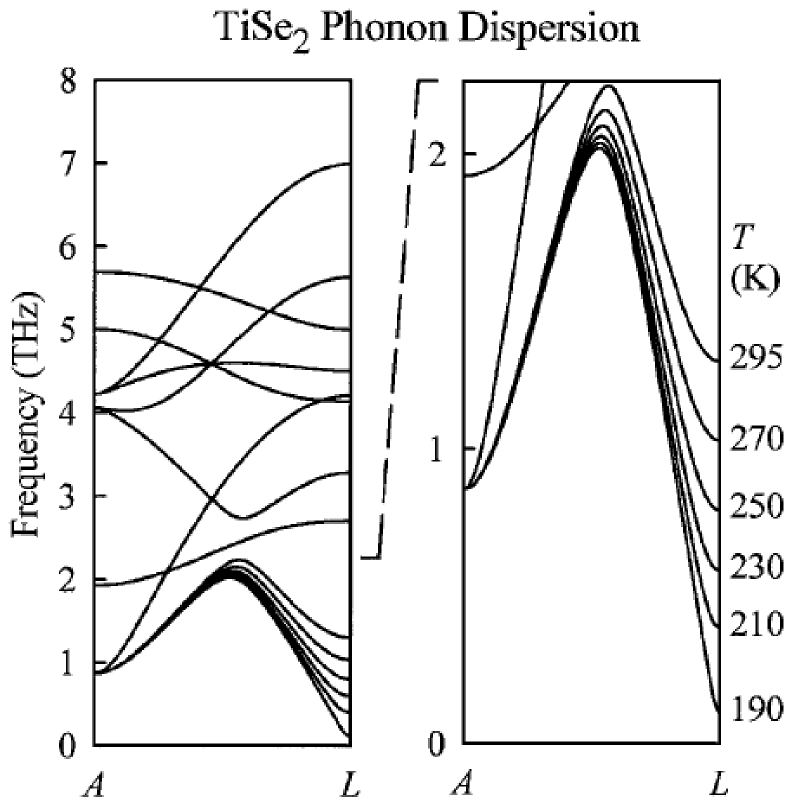
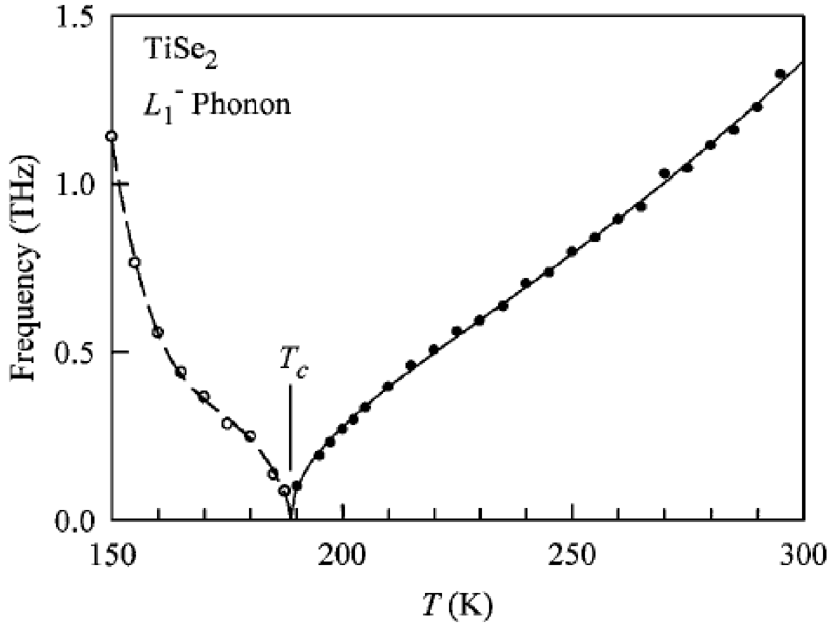
X-Ray Studies of Phonon Softening in $TiSe_2$

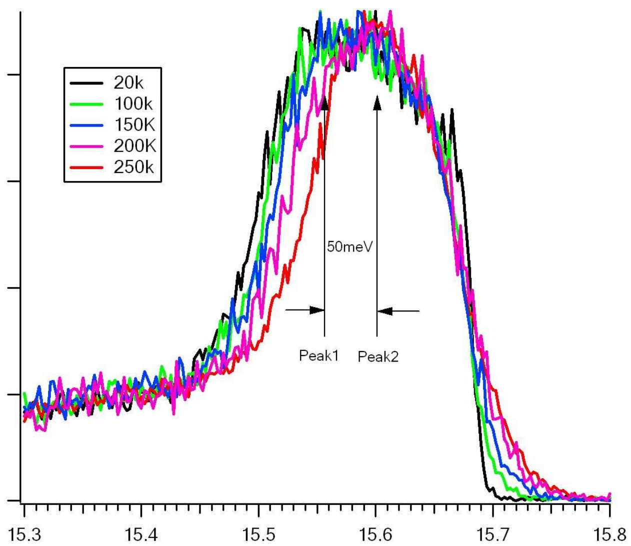
M. Holt,[1,2] P. Zschack,[2] Hawoong Hong,[2] M. Y. Chou,[3] and T.-C. Chiang[1,2,*]



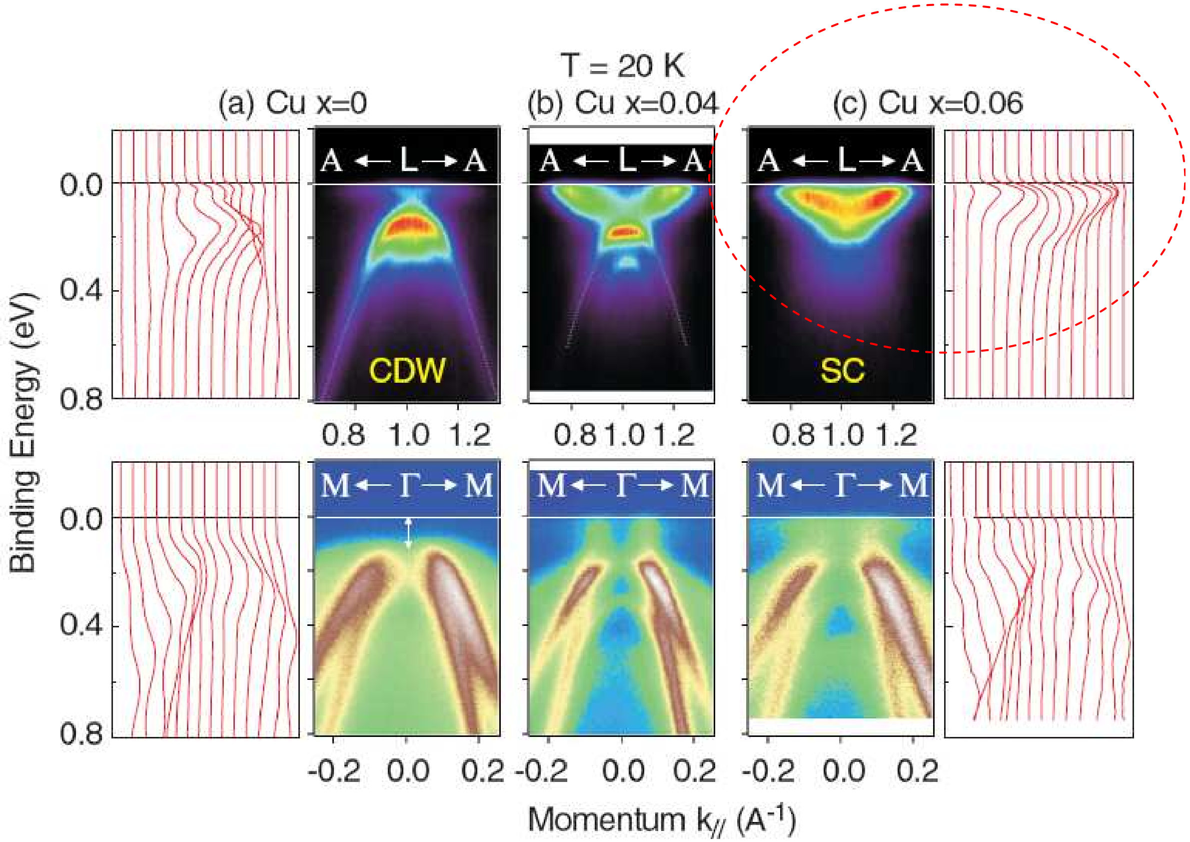


D. Qian et al., PRL (07)

L-point



Kinetic Energy (eV)

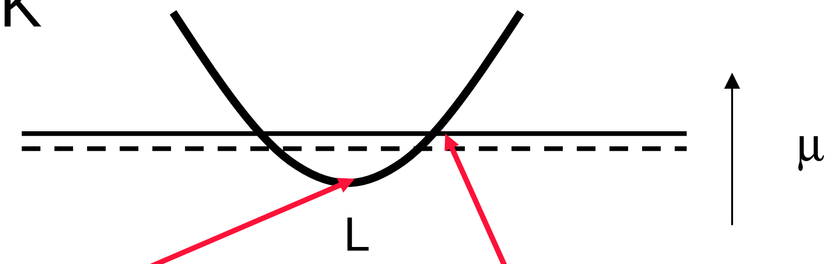


D. Qian et al, unpublished

Possible shift of chemical potential with T

$\mu=\mu_0[1-\alpha(T/T_F)^2]$,

E_F~80-100 meV at 300 K



heavy mass at L point due to very strong electron-phonon scattering, (linked with lattice instability in parent compound).

smaller mass at Fermi crossing point due to reduced scattering (away from L point).

$\Sigma(\varepsilon_k)$ changes along dispersive band!

G. Li et al., PRL (07b)

Summary for CuxTiSe2

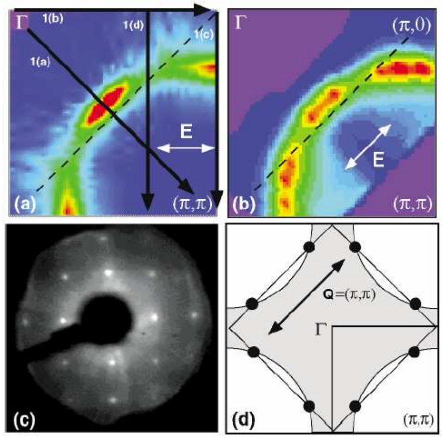
- Semimetal to semimetal CDW transition in 1T-TiSe2.
- Kohn-Overhauser mechanism for CDW phase transition of TiSe2.

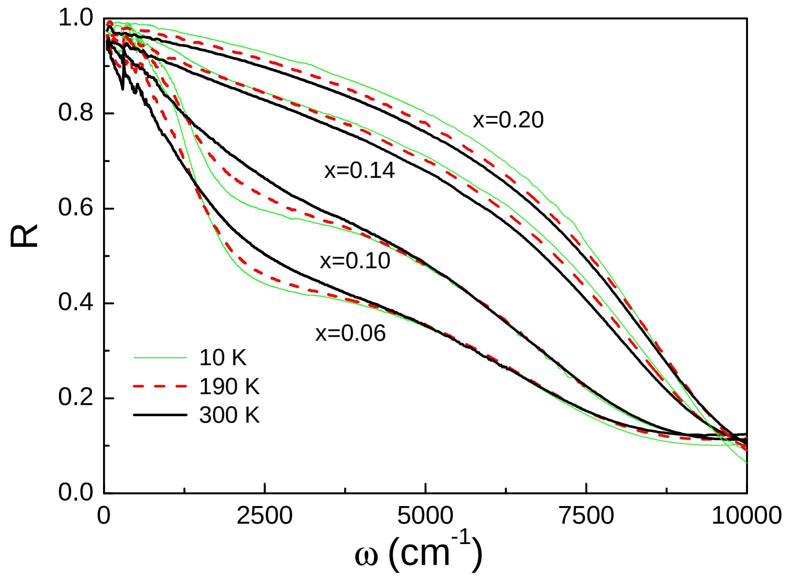
- Cu-intercalation shifts up the chemical potential
- Plasma frequency increases with decreasing T
- T-induced effective mass change.

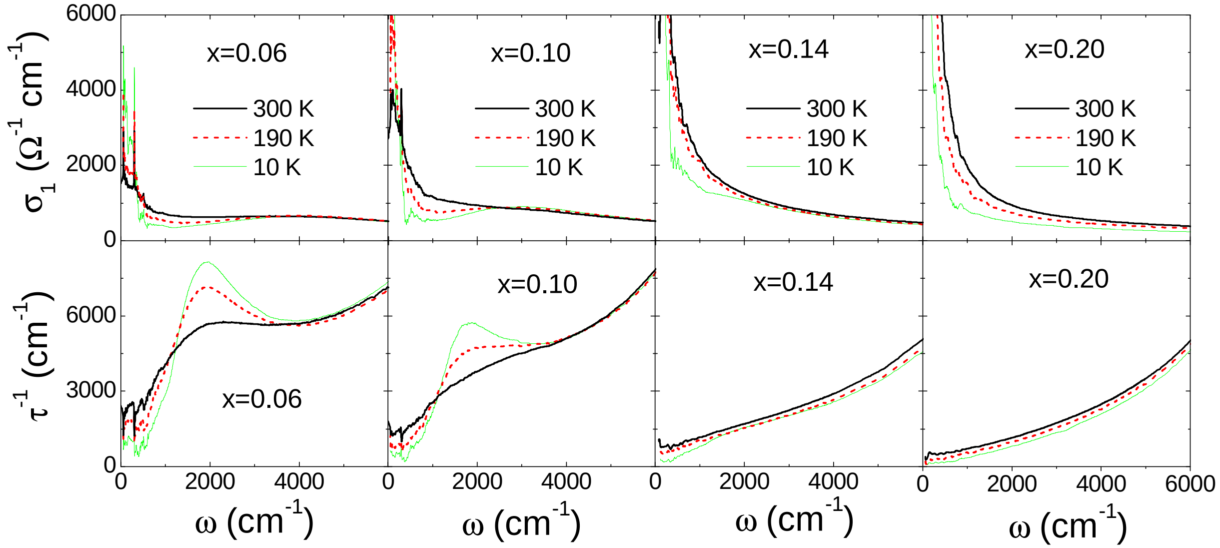
Thank you!!

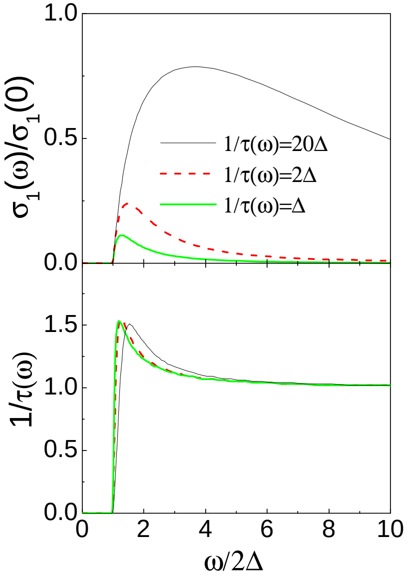
Nd2-xCexCuO4

NL Wang et al. PRB 06









BCS s-wave gap

Low-Temperature Anomalies and Ferromagnetism of EuB_6

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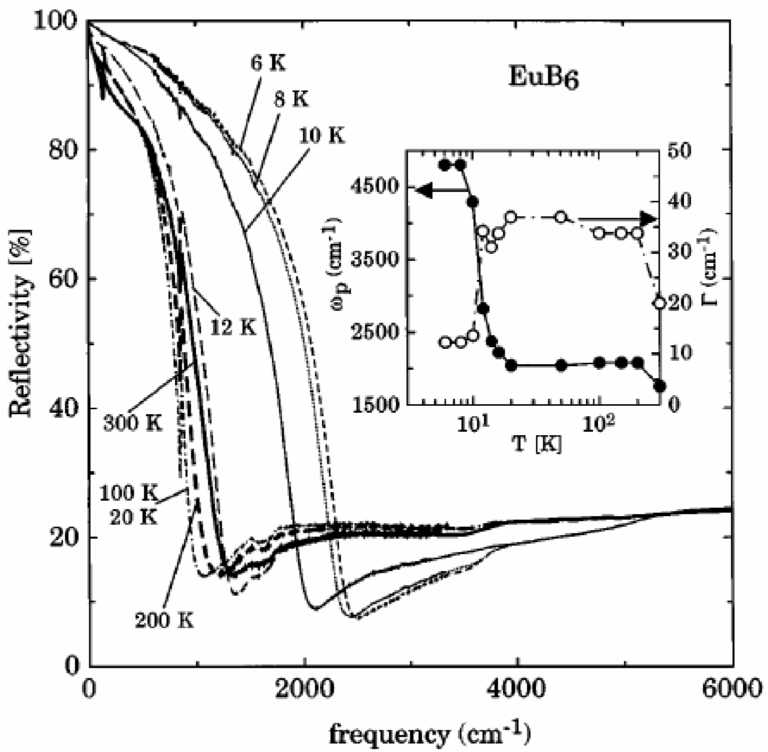
(Received 21 April 1997)



Ferromagnetism from Undressing

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(November 19, 2002)

We have recently proposed that superconductivity may be understood as driven by the undressing of quasiparticles as the superconducting state develops. Similarly we propose here that ferromagnetism in metals may be understood as driven by the undressing of quasiparticles as the ferromagnetic state develops. In ferromagnets, the undressing is proposed to occur due to the reduction in *bond charge* caused by spin polarization, in contrast to superconductors where the undressing is proposed to occur due to the reduction in *site charge* caused by (hole) pairing. The undressing process manifests itself in the one and two-particle Green's functions as a transfer of spectral weight from high to low frequencies. Hence it should have universal observable consequences in one- and two-particle spectroscopies such as photoemission and optical absorption.

Cond-mat/0007454 (PRB (2000))