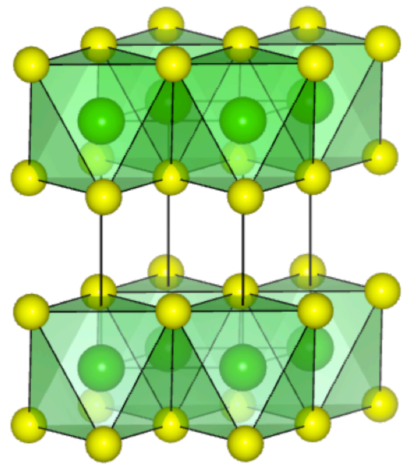
ABSENCE OF CDW AND POSSIBLE ELECTRONIC INSTABILITY IN 2D VS_2

Andrea Gauzzi

Institut de Minéralogie et de Physique des Milieux Condensés
UPMC – Sorbonne Universités and CNRS, Paris



GDR-MICO, Roscoff, 7-10 January 2013

COLLABORATORS

A. Sellam, G. Rousse, Y. Klein, P. Giura, D. Taverna, M. Calandra, G. Loupias IMPMC, Paris

F. Gozzo, SLS, Villigen

E.Gilioli, F. Bolzoni, G.L. Calestani, Parme

P. Roy, AILES-SOLEIL

D. Pelloquin, Caen

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E. Tosatti, H. Takagi, R. Lobo, B. Leridon

OUTLINE

- Introduction and motivation
  - Dichalcogenides 2D MX_2: CDW-SC interplay

- 1T-VS_2: little studied
  - Metastability
  - Previous studies: evidence of CDW and metallic properties

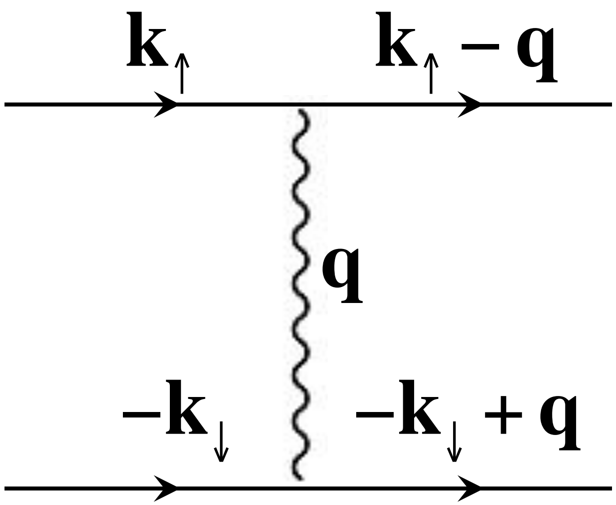
- Structural and physical properties of 1T-VS_2
  - High-pressure synthesis
  - Discrepancies with previous works: absence of CDW
  - Hint of electronic instability

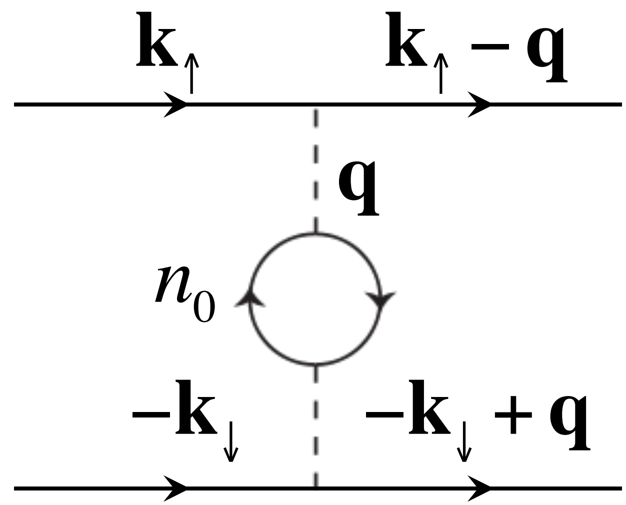
- Conclusions and perspectives

SEARCH FOR EXCITONIC SUPERCONDUCTIVITY

Pioonering works:

1. W.A. Little, Phys. Rev. **134**, A1416 (1964).
2. V. Ginzburg, Sov. Phys. JETP **20**, 1549 (1965).





Conventional BCS:
exchange of virtual phonon

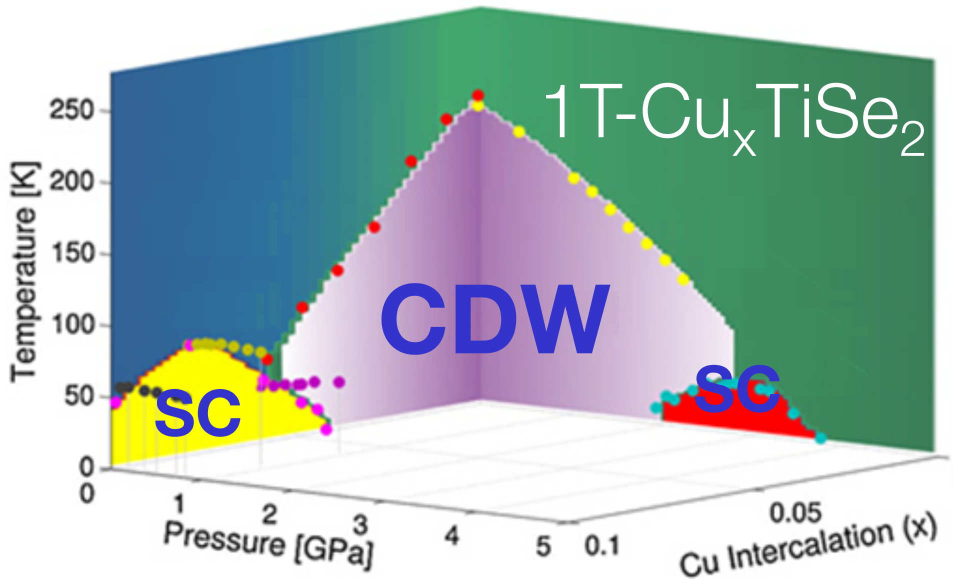
Excitonic BCS:
exchange of virtual photon

- Favourable condition: weakly screened 2D semi-metals

★ 2D MX_2 (X=S, Se) compounds are good candidates

INTERPLAY BETWEEN SC-CDW IN 2D MX_2 SYSTEM

- Which microscopic mechanism(s) for SC and CDW?



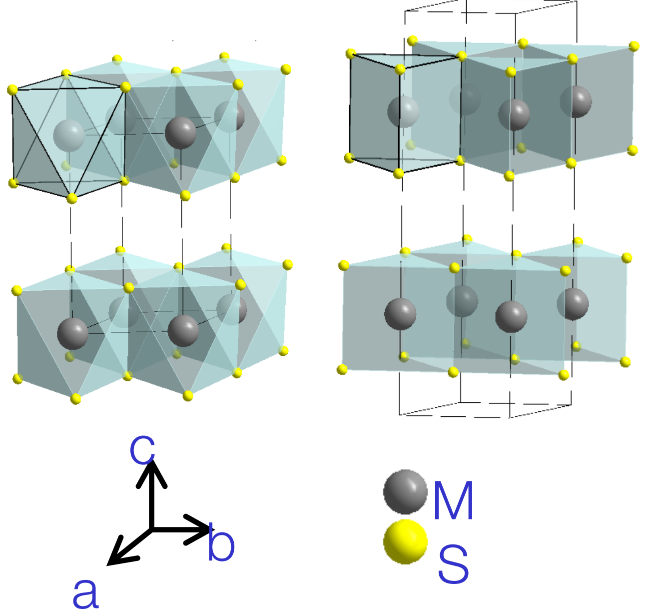
Kusmartseva et al. (2009)

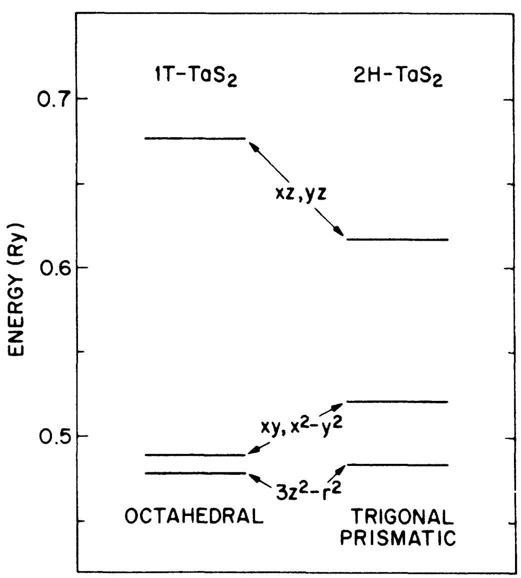
Controversial scenarios:

1. Fermi surface nesting (Peierls mechanism)
2. Exciton condensate
3. Electron-phonon coupling
4. RVB mechanism (see also cuprates)

POLYTYPES AND STABILITY OF MS_2 COMPOUNDS

1T (P-3*m*1) 2H (P6_3/*mmc*)





- 1T and 2H main polytypes
- 1T and 2H: similar total energy but different electronic structures
- **1T-VS_2:** hitherto reported only by de-intercalation of Li in $LiVS_2$ (Murphy et al., 1977)

d^0	d^1	d^2
Ti	V	Cr
Zr	Nb	Mo
Hf	Ta	W

- 1T stable
- 2H stable
- 1T-VS_2: metastable
- CrS_2: not reported yet

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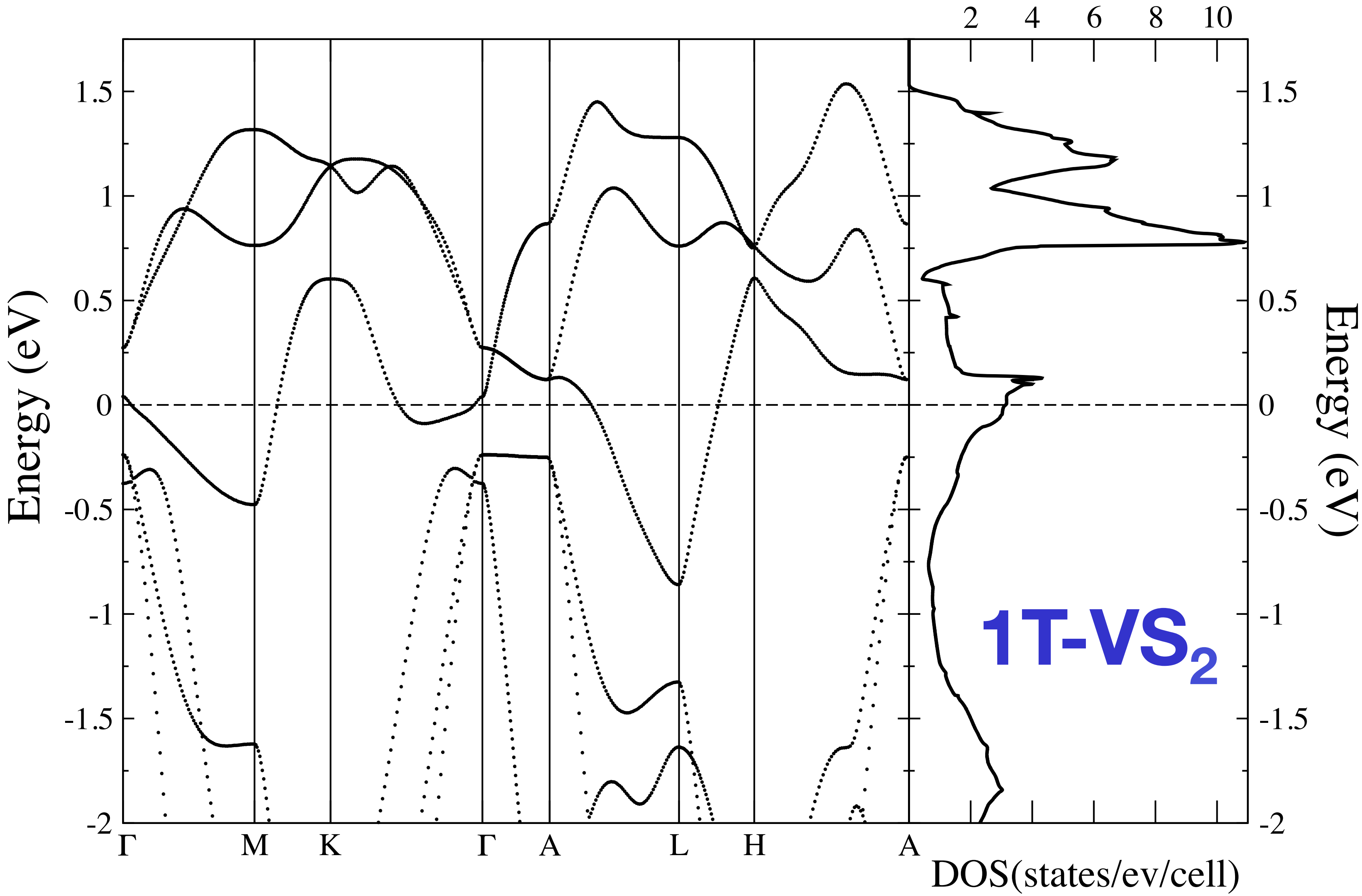
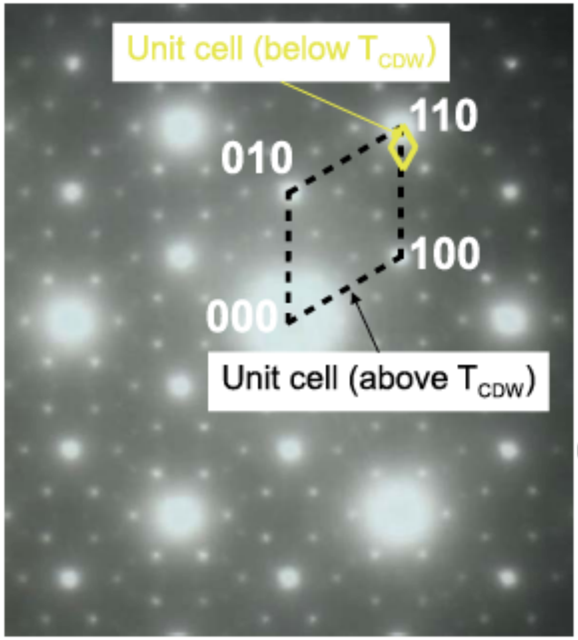
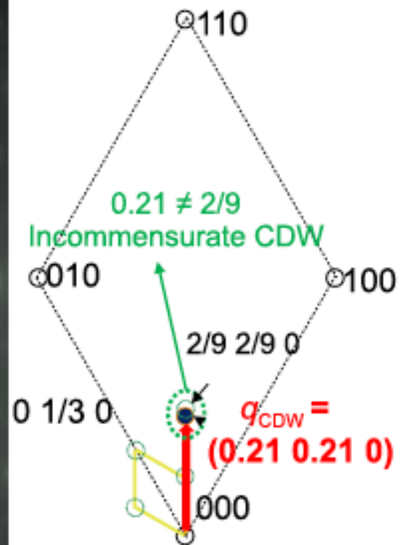
ELECTRONIC STRUCTURE OF 1T-MS_2 COMPOUNDS
SEMIMETALLIC CHARACTER

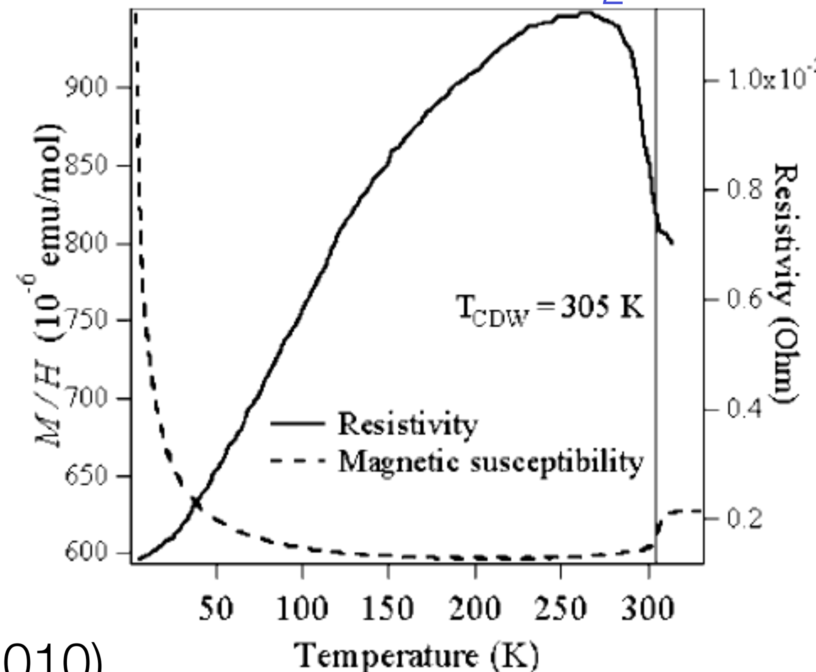


Gauzzi et al. (unpublished)

PREVIOUS WORK: OBSERVATION OF CDW IN VS_2



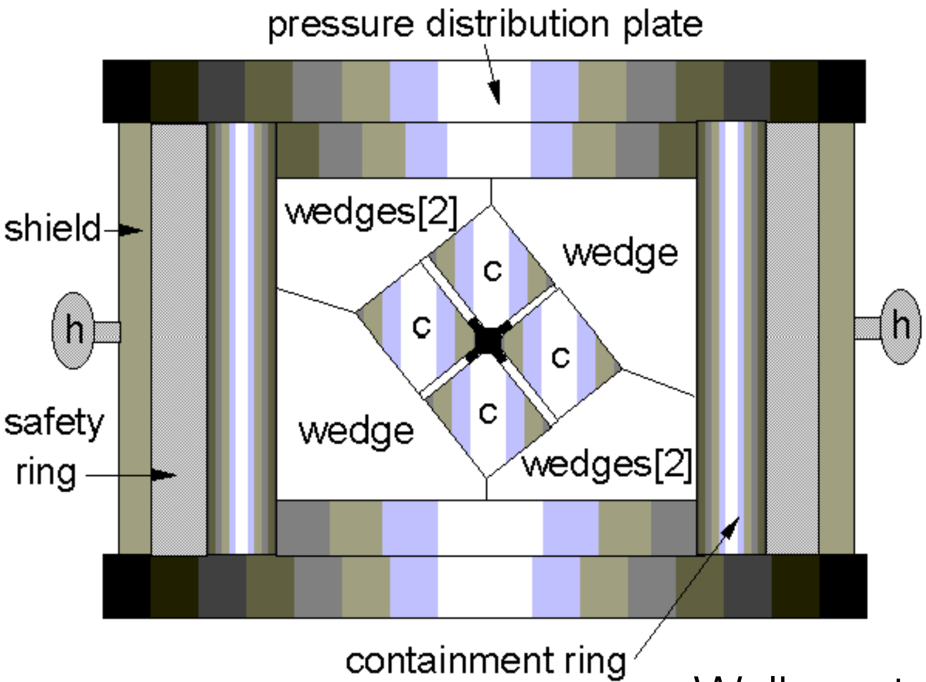


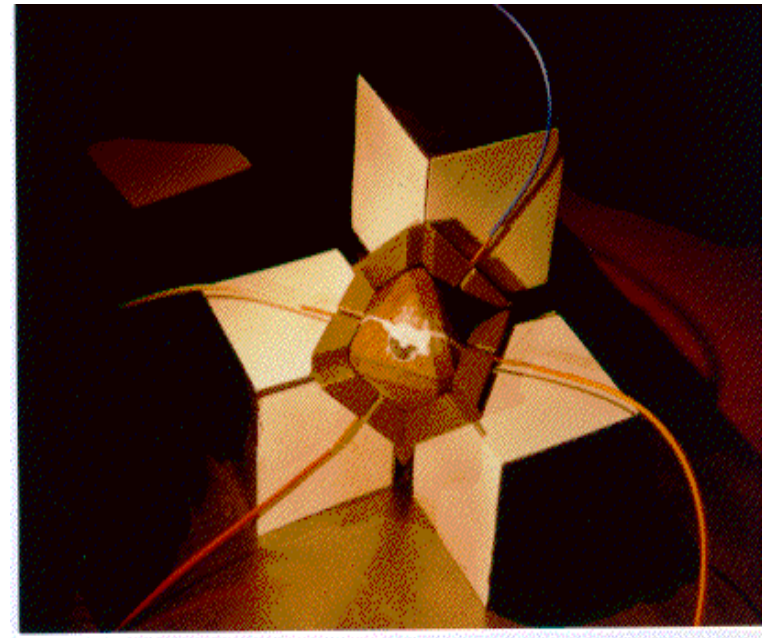


Mulazzi et al. (2010)

- $3d^1$ configuration of V ion confirmed by RPES
- Incommensurate CDW below T_{CDW}=305 K
- Fermi nesting scenario ruled out
- Phonon softening scenario with fairly large λ=0.45
- Metallic behaviour with ρ_{300K}~1mΩcm

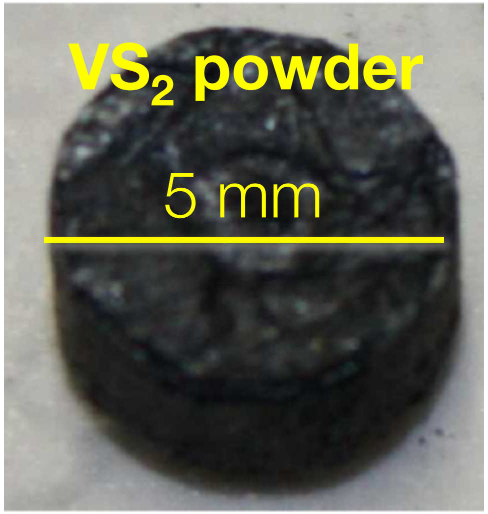
MULTI-ANVIL HIGH-PRESSURE SYNTHESIS OF VS_2



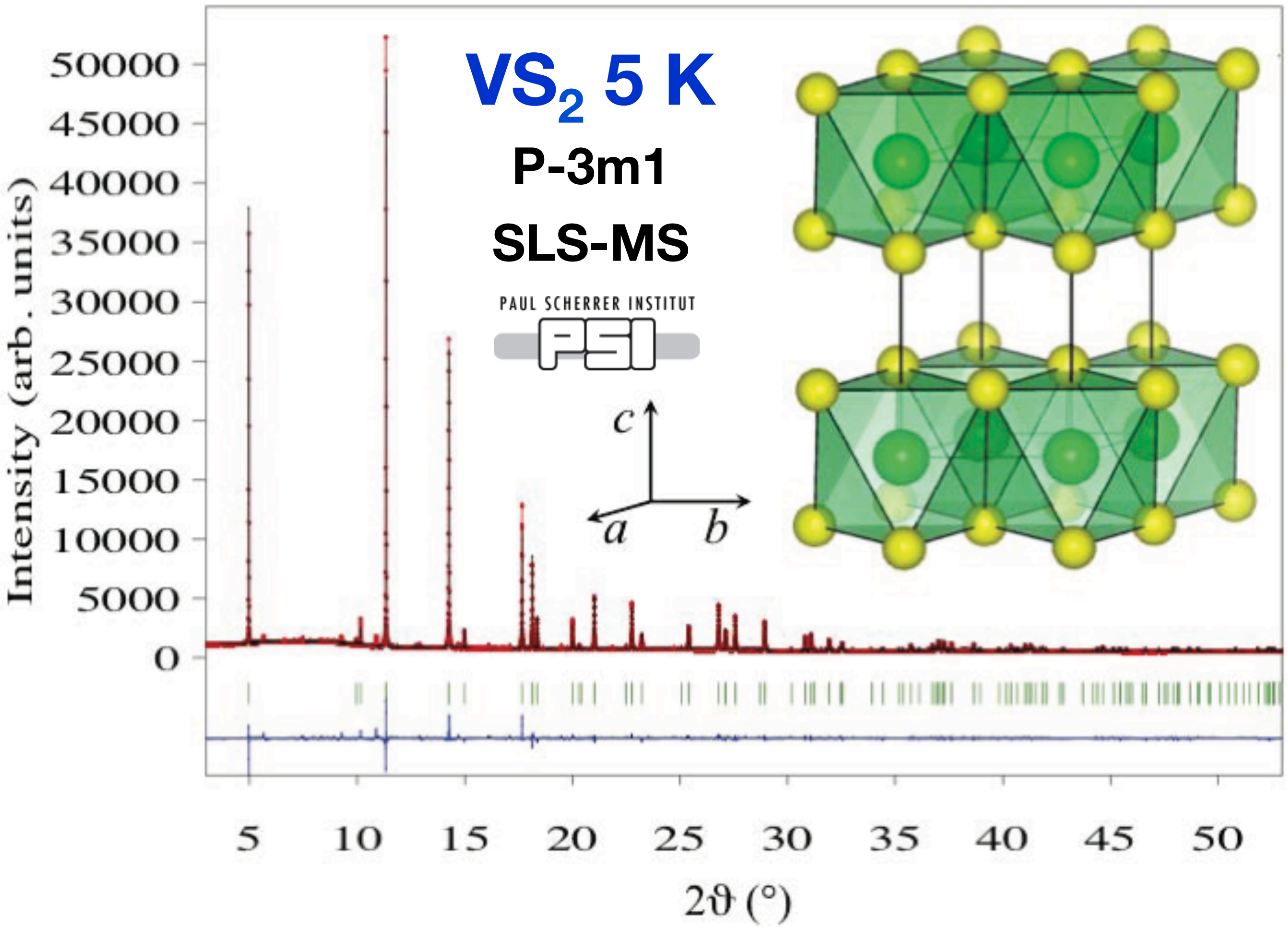


Walker et al. (1991)

- Very high quasi-hydrostatic *P* up to 25 GPa
- Synthesis of 1T-VS_2:
  - $P = 4$ GPa
  - $T = 700$ °C
- Sintered powder samples > 95% pure
- "Large" samples V~100 mm^3



STRUCTURAL REFINEMENT OF 1T-VS_2

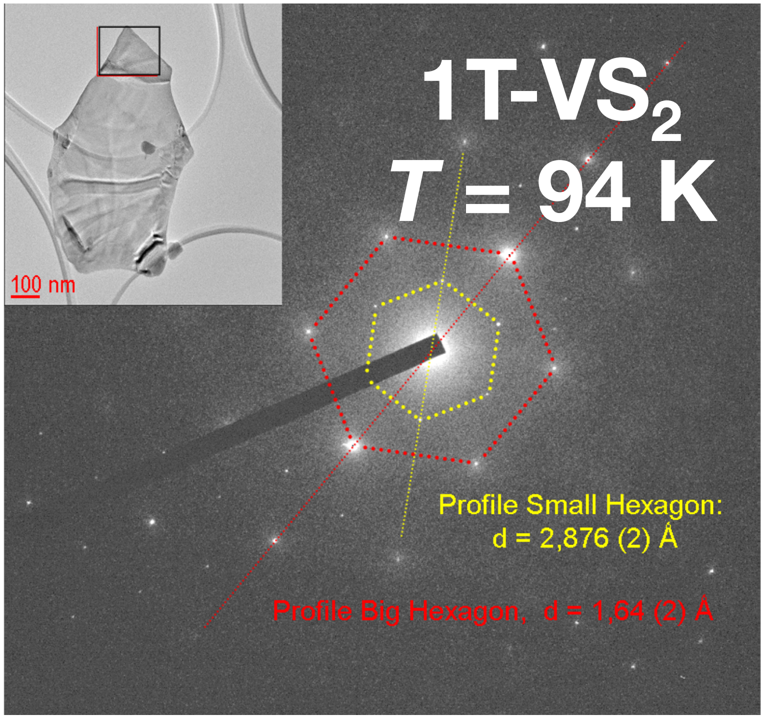


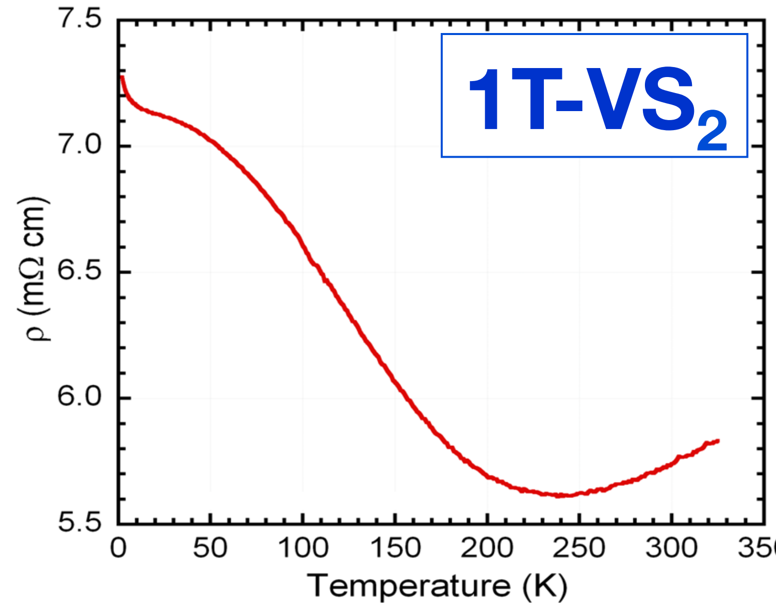
This work (300 K):
a = 3.2495(1) Å; *c* = 5.7038(2) Å

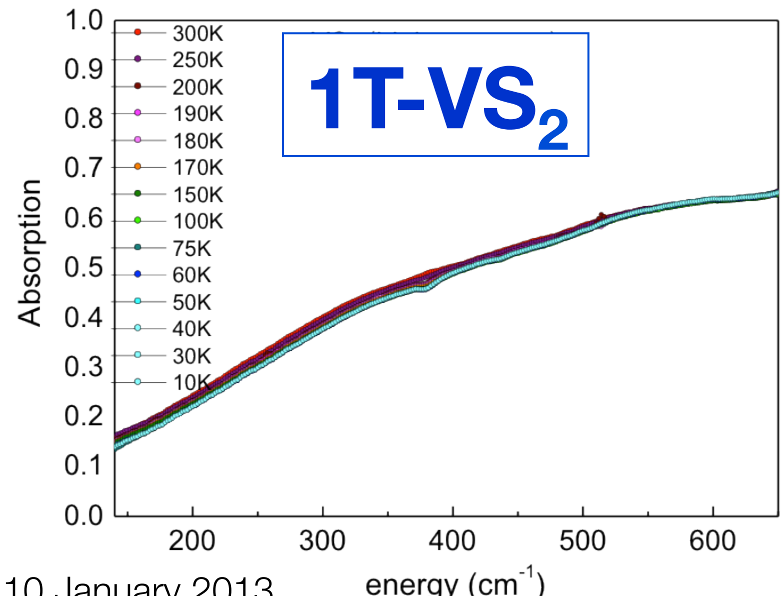
Murphy et al. (1977) (300 K)
a = 3.217 Å; *c* = 5.755 Å

★ HP synthesis leads to ~1% changes of lattice parameters

ABSENCE OF CDW AND SEMIMETALLIC PROPERTIES OF 1T-VS_2 SYNTHESISED UNDER HIGH PRESSURE







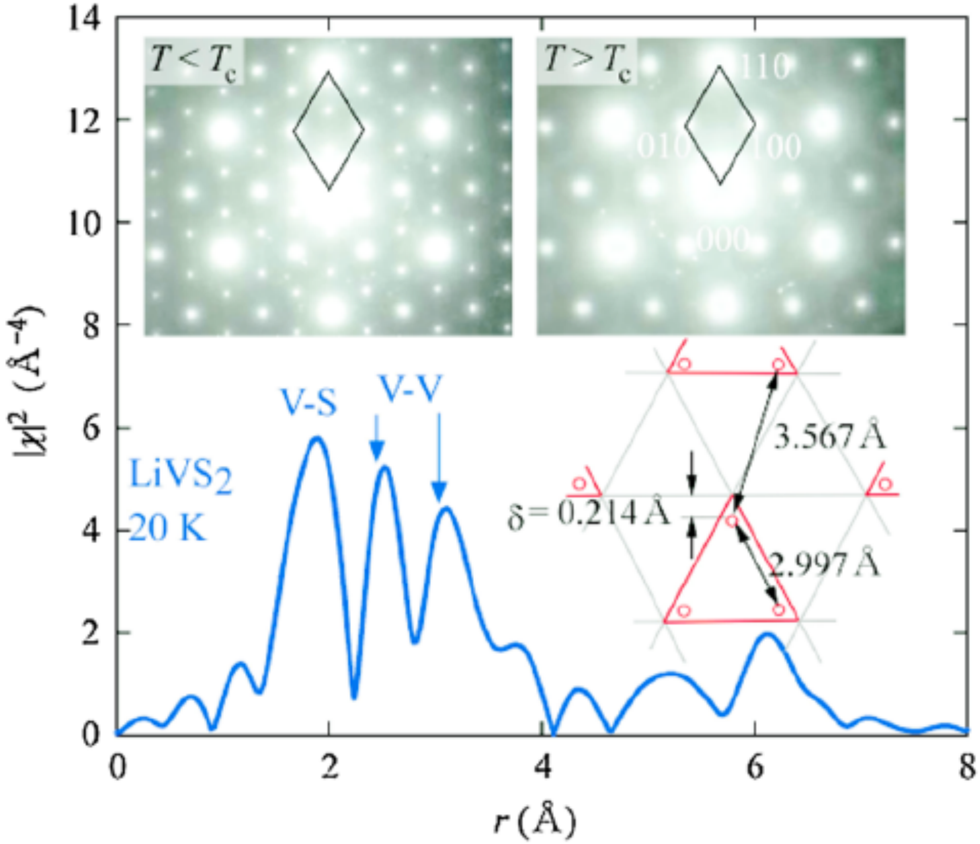
Discrepancies with Li de-intercalated samples:

- ★ No CDW at any temperature
- ★ Semimetallic behaviour of $\rho(T)$ and IR optical conductivity $\sigma_\omega(T)$

POSSIBLE EXPLANATION OF DISCREPANCY

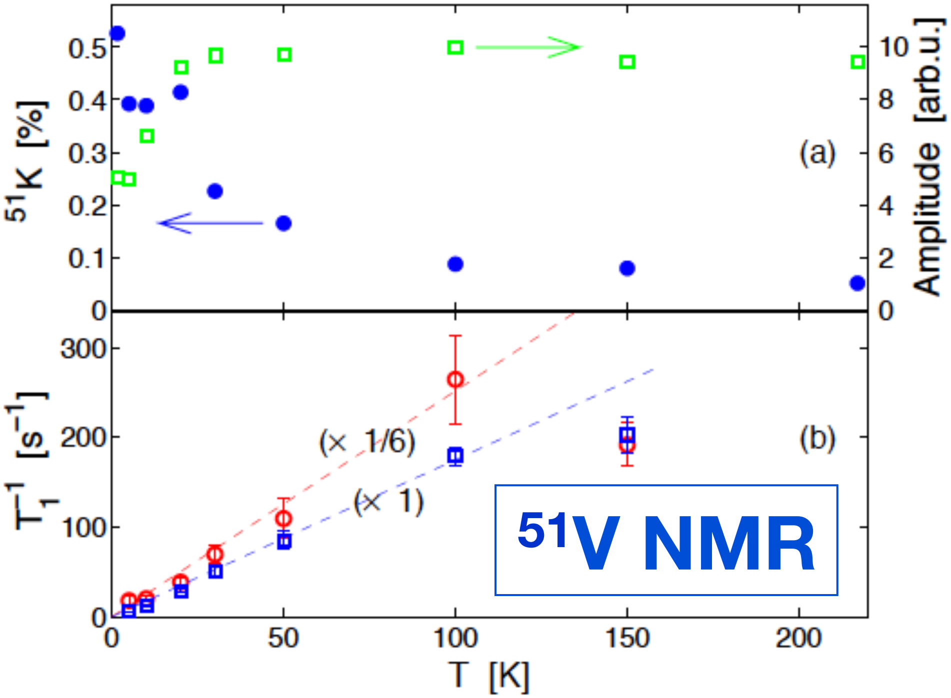
Li de-intercalated Li_xVS_2 samples contains residual Li?

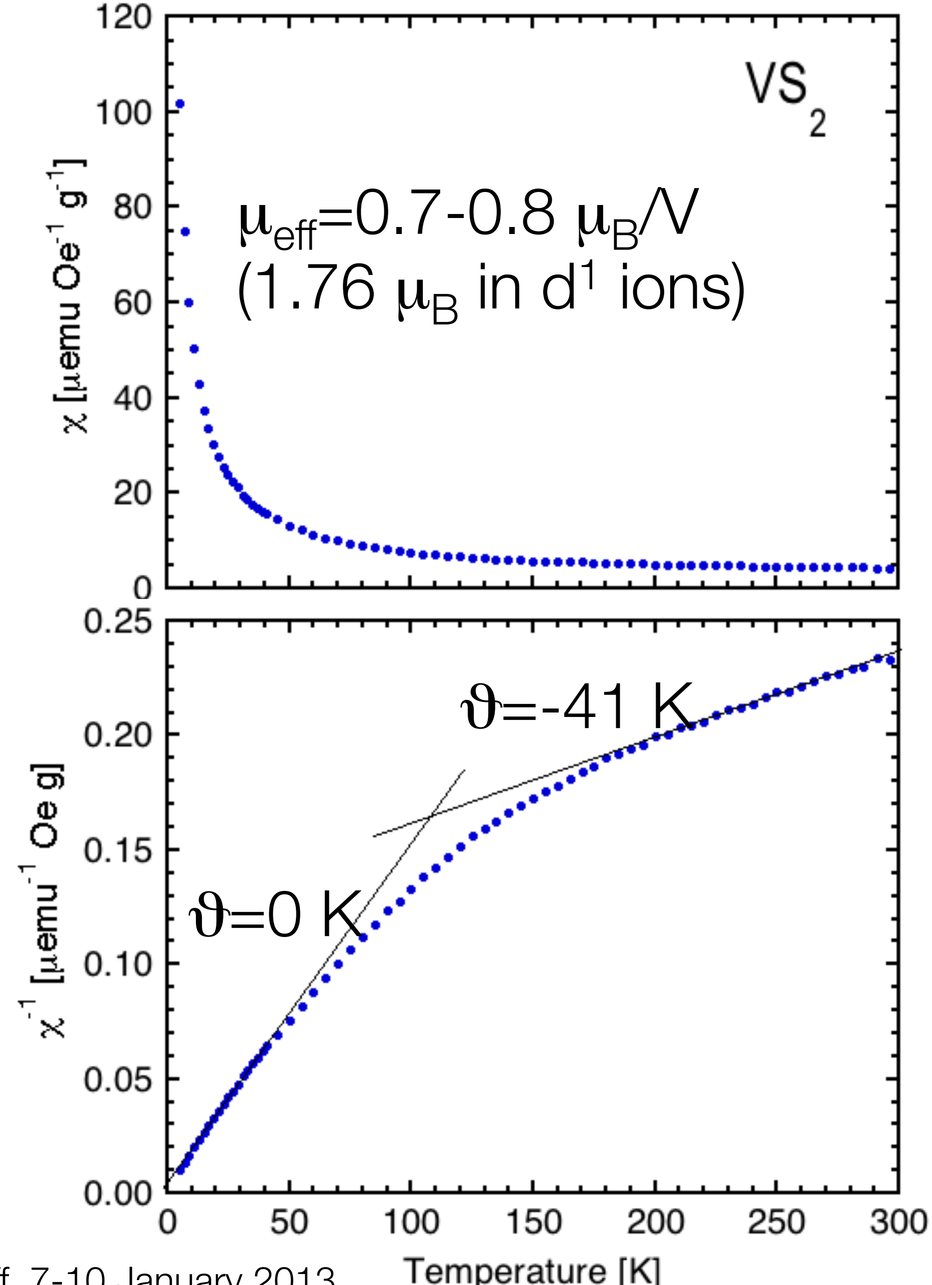
Hint: observation of orbital ordering (Valence Bond Solid at T_c=305 K in $LiVS_2$ leading to V trimerisation.



Katayama et al. (2009)

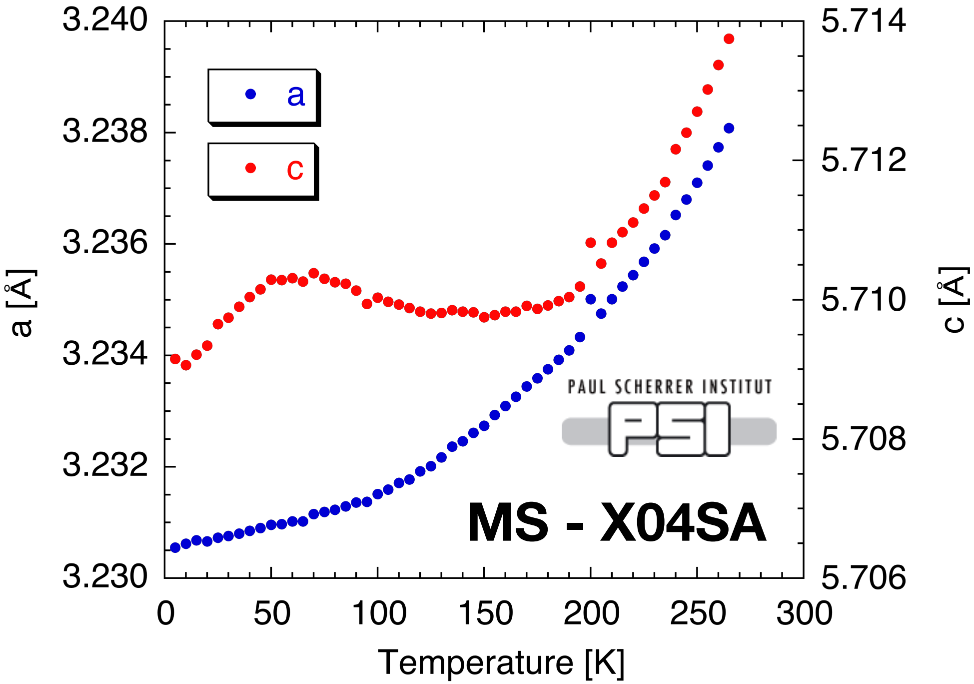
1T-VS_2: MAGNETIC RESPONSE

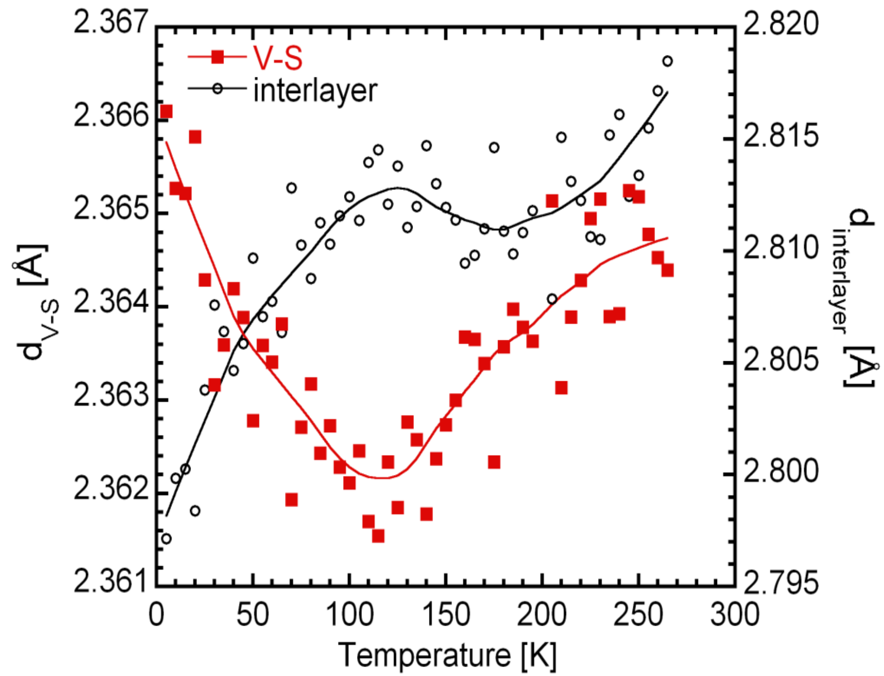




- ~7% of localised V moments
- Dominant Pauli contribution
- Behaviour of $1/T_1$: Korringa law (non-magnetic metal)
- Crossover at ~100 K: from AF-like to vanishing ϑ and larger $1/T_2$

EVIDENCE OF STRUCTURAL ANOMALY IN 1T-VS_2





- Negative thermal expansion of c-axis in the 50-150 K range (~4 pm increase with respect to extrapolated Debye behaviour)
- Negative thermal expansion of V-S bond distance below 100 K (~8 pm increase)

★ Electronic instability (charge fluctuation?) of V^{4+} ion?

CONCLUSIONS

- Successful HP synthesis of pure 1T-VS_2 powders
- Absence of CDW (discrepancy with Li de-intercalated samples)
- Further discrepancy concerns semimetallic behaviour
- 1T-VS_2 is a non-magnetic semi-metal
- Crossover of magnetic response below ~100 K
(likely enhanced spin-spin relaxation rate)
- Crossover concomitant to negative *c*-axis thermal expansion
(increase of V-V distance below ~100 K)

PERSPECTIVES AND FUTURE WORK

- High-pressure growth of single-crystals
- EPR study to probe the *T*-dependent localised moments
- Link between magnetic crossover and structural anomaly
- Is 1T-VS_2 far from a superconducting instability?